



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 08:44 PM UTC

PDB ID : 2HD0 / pdb_00002hd0
Title : Structure of the catalytic domain of hepatitis C virus NS2
Authors : Lorenz, I.C.; Rice, C.M.; Marcotrigiano, J.
Deposited on : 2006-06-19
Resolution : 2.28 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

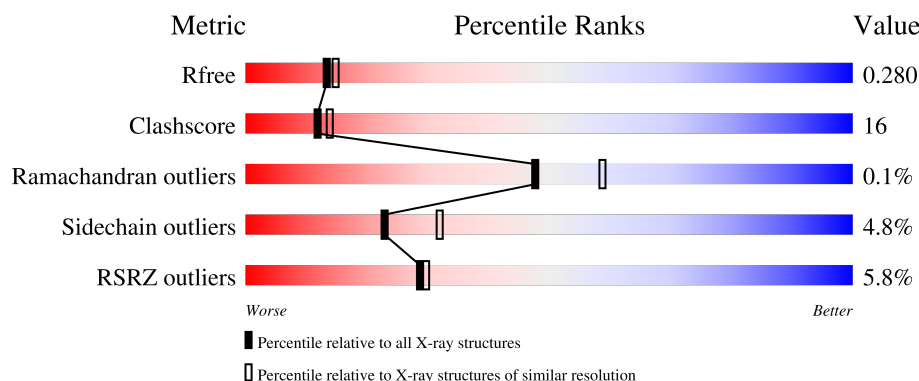
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.28 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	128	2% 66% 30% ..
1	B	128	4% 72% 25% ..
1	C	128	2% 68% 29% ..
1	D	128	8% 70% 28% ...
1	E	128	% 67% 30% ..

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Mol	Chain	Length	Quality of chain
1	F	128	
1	G	128	
1	H	128	
1	I	128	
1	J	128	
1	K	128	
1	L	128	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DMU	I	218	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11930 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Protease NS2-3 (p23).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	127	Total	C	N	O	S	0	0	0
			974	625	177	166	6			
1	B	127	Total	C	N	O	S	0	0	0
			958	616	170	166	6			
1	C	127	Total	C	N	O	S	0	0	0
			966	620	175	165	6			
1	D	127	Total	C	N	O	S	0	0	0
			958	618	172	162	6			
1	E	127	Total	C	N	O	S	0	0	0
			964	620	174	164	6			
1	F	127	Total	C	N	O	S	0	0	0
			950	611	168	165	6			
1	G	127	Total	C	N	O	S	0	0	0
			951	613	169	163	6			
1	H	128	Total	C	N	O	S	0	0	0
			958	617	170	165	6			
1	I	127	Total	C	N	O	S	0	0	0
			952	613	167	166	6			
1	J	127	Total	C	N	O	S	0	0	0
			970	622	176	166	6			
1	K	127	Total	C	N	O	S	0	0	0
			948	611	167	164	6			
1	L	127	Total	C	N	O	S	0	0	0
			952	614	167	165	6			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP P27958
A	2	SER	-	cloning artifact	UNP P27958
A	3	HIS	-	cloning artifact	UNP P27958
A	4	MET	-	cloning artifact	UNP P27958
A	139	TYR	CYS	variant	UNP P27958

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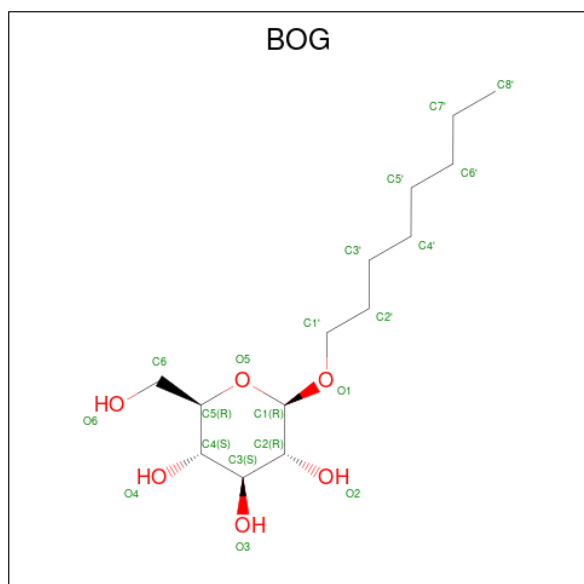
Chain	Residue	Modelled	Actual	Comment	Reference
A	145	THR	ALA	variant	UNP P27958
B	1	GLY	-	cloning artifact	UNP P27958
B	2	SER	-	cloning artifact	UNP P27958
B	3	HIS	-	cloning artifact	UNP P27958
B	4	MET	-	cloning artifact	UNP P27958
B	139	TYR	CYS	variant	UNP P27958
B	145	THR	ALA	variant	UNP P27958
C	1	GLY	-	cloning artifact	UNP P27958
C	2	SER	-	cloning artifact	UNP P27958
C	3	HIS	-	cloning artifact	UNP P27958
C	4	MET	-	cloning artifact	UNP P27958
C	139	TYR	CYS	variant	UNP P27958
C	145	THR	ALA	variant	UNP P27958
D	1	GLY	-	cloning artifact	UNP P27958
D	2	SER	-	cloning artifact	UNP P27958
D	3	HIS	-	cloning artifact	UNP P27958
D	4	MET	-	cloning artifact	UNP P27958
D	139	TYR	CYS	variant	UNP P27958
D	145	THR	ALA	variant	UNP P27958
E	1	GLY	-	cloning artifact	UNP P27958
E	2	SER	-	cloning artifact	UNP P27958
E	3	HIS	-	cloning artifact	UNP P27958
E	4	MET	-	cloning artifact	UNP P27958
E	139	TYR	CYS	variant	UNP P27958
E	145	THR	ALA	variant	UNP P27958
F	1	GLY	-	cloning artifact	UNP P27958
F	2	SER	-	cloning artifact	UNP P27958
F	3	HIS	-	cloning artifact	UNP P27958
F	4	MET	-	cloning artifact	UNP P27958
F	139	TYR	CYS	variant	UNP P27958
F	145	THR	ALA	variant	UNP P27958
G	1	GLY	-	cloning artifact	UNP P27958
G	2	SER	-	cloning artifact	UNP P27958
G	3	HIS	-	cloning artifact	UNP P27958
G	4	MET	-	cloning artifact	UNP P27958
G	139	TYR	CYS	variant	UNP P27958
G	145	THR	ALA	variant	UNP P27958
H	1	GLY	-	cloning artifact	UNP P27958
H	2	SER	-	cloning artifact	UNP P27958
H	3	HIS	-	cloning artifact	UNP P27958
H	4	MET	-	cloning artifact	UNP P27958
H	139	TYR	CYS	variant	UNP P27958

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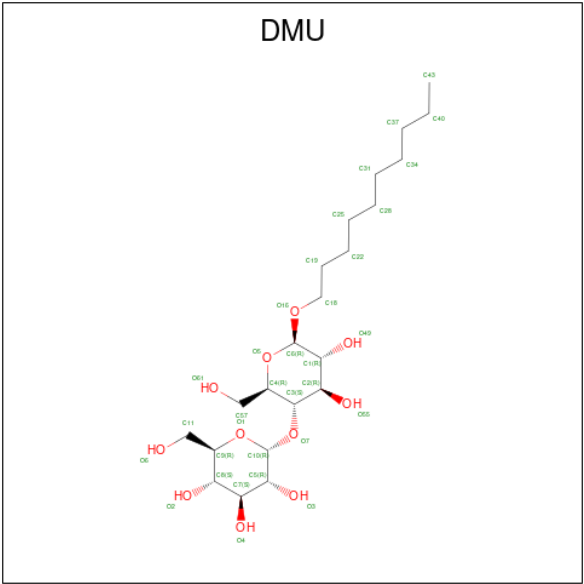
Chain	Residue	Modelled	Actual	Comment	Reference
H	145	THR	ALA	variant	UNP P27958
I	1	GLY	-	cloning artifact	UNP P27958
I	2	SER	-	cloning artifact	UNP P27958
I	3	HIS	-	cloning artifact	UNP P27958
I	4	MET	-	cloning artifact	UNP P27958
I	139	TYR	CYS	variant	UNP P27958
I	145	THR	ALA	variant	UNP P27958
J	1	GLY	-	cloning artifact	UNP P27958
J	2	SER	-	cloning artifact	UNP P27958
J	3	HIS	-	cloning artifact	UNP P27958
J	4	MET	-	cloning artifact	UNP P27958
J	139	TYR	CYS	variant	UNP P27958
J	145	THR	ALA	variant	UNP P27958
K	1	GLY	-	cloning artifact	UNP P27958
K	2	SER	-	cloning artifact	UNP P27958
K	3	HIS	-	cloning artifact	UNP P27958
K	4	MET	-	cloning artifact	UNP P27958
K	139	TYR	CYS	variant	UNP P27958
K	145	THR	ALA	variant	UNP P27958
L	1	GLY	-	cloning artifact	UNP P27958
L	2	SER	-	cloning artifact	UNP P27958
L	3	HIS	-	cloning artifact	UNP P27958
L	4	MET	-	cloning artifact	UNP P27958
L	139	TYR	CYS	variant	UNP P27958
L	145	THR	ALA	variant	UNP P27958

- Molecule 2 is octyl beta-D-glucopyranoside (CCD ID: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			20	14	6		
2	A	1	Total	C	O	0	0
			20	14	6		
2	A	1	Total	C	O	0	0
			20	14	6		
2	B	1	Total	C	O	0	0
			20	14	6		
2	C	1	Total	C	O	0	0
			20	14	6		
2	F	1	Total	C	O	0	0
			20	14	6		
2	F	1	Total	C	O	0	0
			20	14	6		
2	H	1	Total	C	O	0	0
			20	14	6		
2	I	1	Total	C	O	0	0
			20	14	6		
2	J	1	Total	C	O	0	0
			20	14	6		
2	K	1	Total	C	O	0	0
			20	14	6		

- Molecule 3 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: $C_{22}H_{42}O_{11}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	I	1	Total	C	O	0	0
			33	22	11		

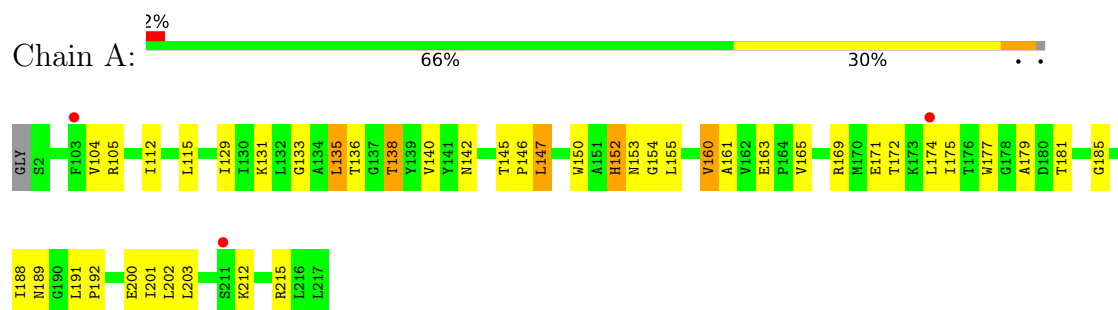
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	16	Total	O	0	0
			16	16		
4	B	10	Total	O	0	0
			10	10		
4	C	24	Total	O	0	0
			24	24		
4	D	14	Total	O	0	0
			14	14		
4	E	29	Total	O	0	0
			29	29		
4	F	13	Total	O	0	0
			13	13		
4	G	15	Total	O	0	0
			15	15		
4	H	13	Total	O	0	0
			13	13		
4	I	14	Total	O	0	0
			14	14		
4	J	8	Total	O	0	0
			8	8		
4	K	13	Total	O	0	0
			13	13		
4	L	7	Total	O	0	0
			7	7		

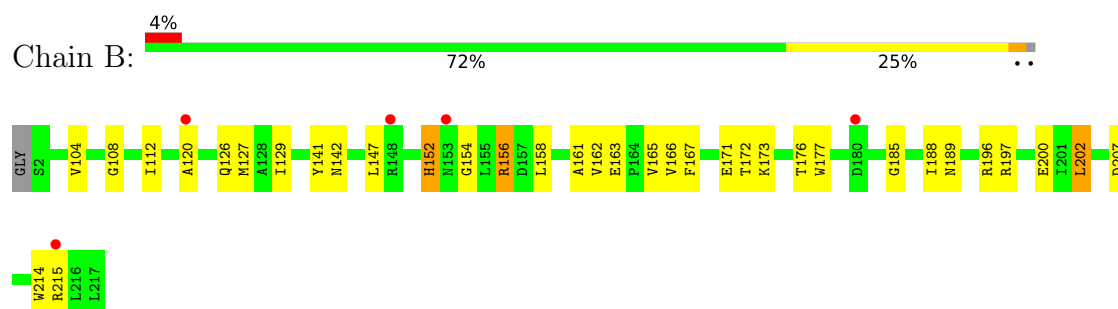
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

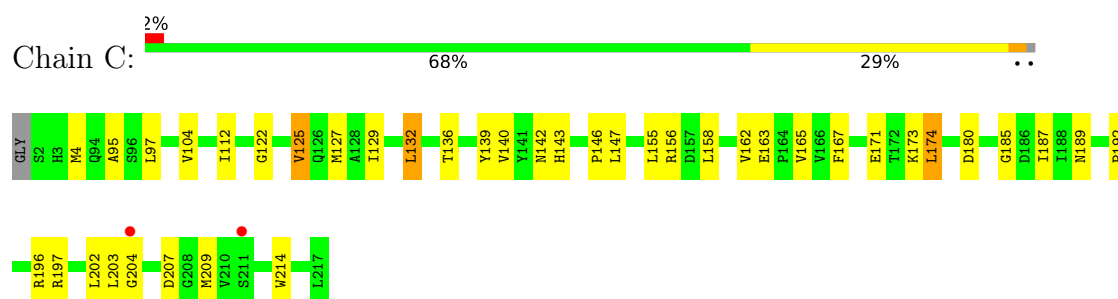
- Molecule 1: Protease NS2-3 (p23)



- Molecule 1: Protease NS2-3 (p23)

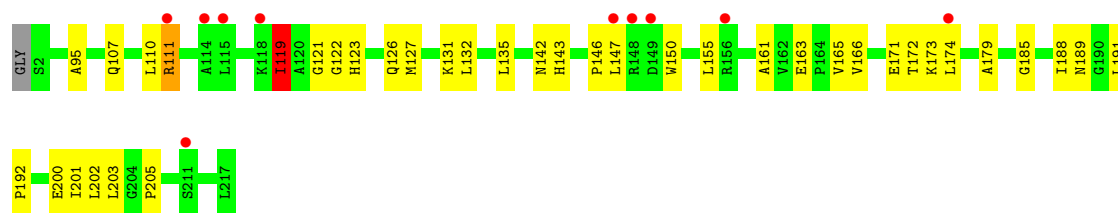


- Molecule 1: Protease NS2-3 (p23)

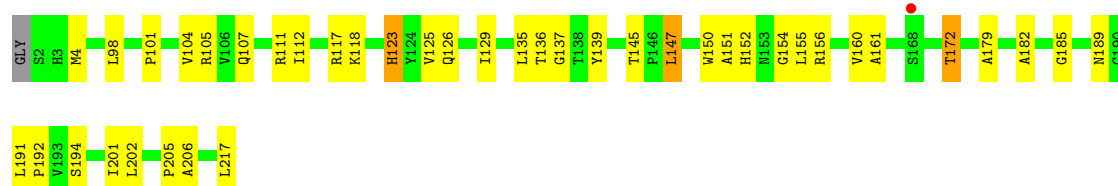


- Molecule 1: Protease NS2-3 (p23)

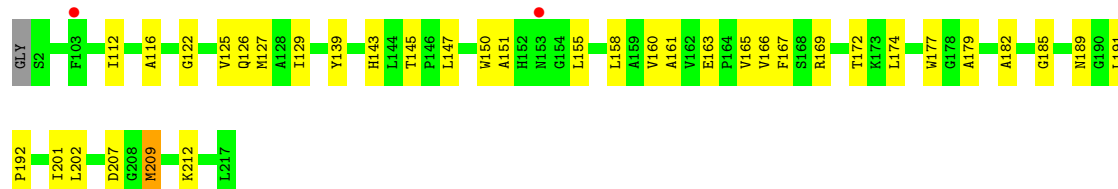




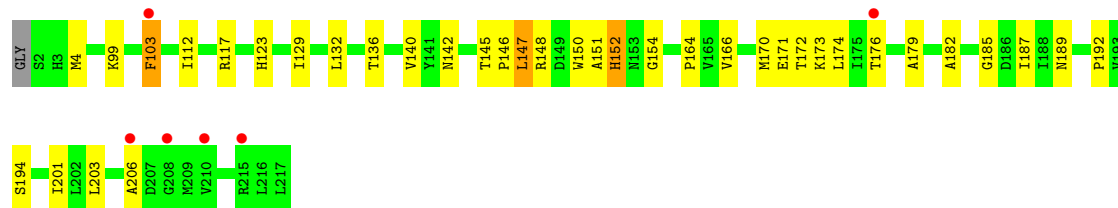
• Molecule 1: Protease NS2-3 (p23)



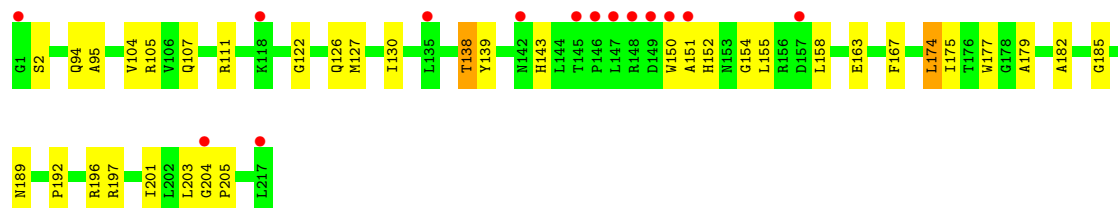
• Molecule 1: Protease NS2-3 (p23)



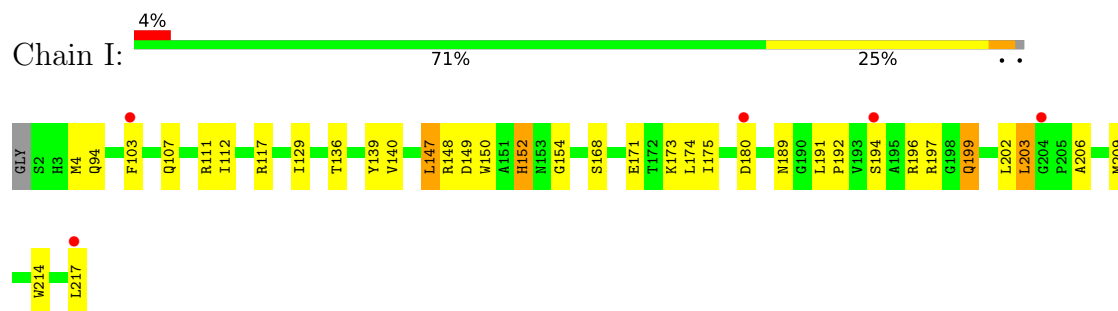
• Molecule 1: Protease NS2-3 (p23)



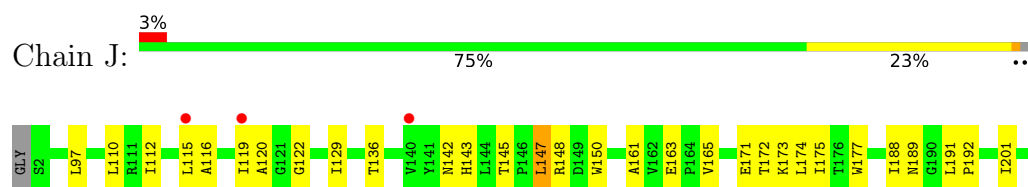
• Molecule 1: Protease NS2-3 (p23)



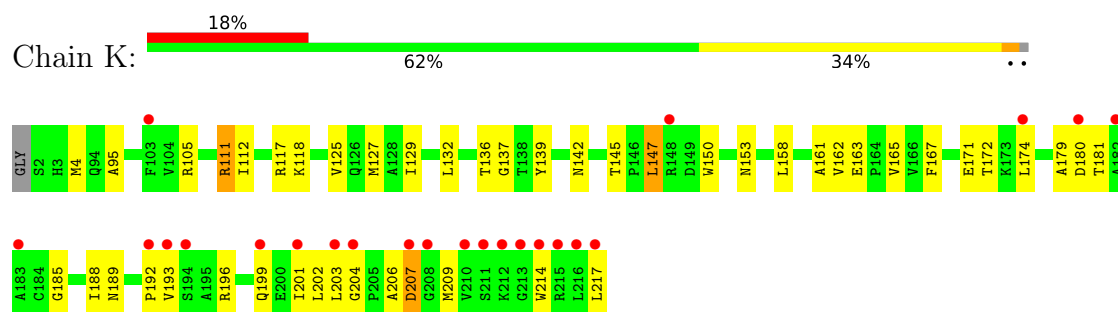
- Molecule 1: Protease NS2-3 (p23)



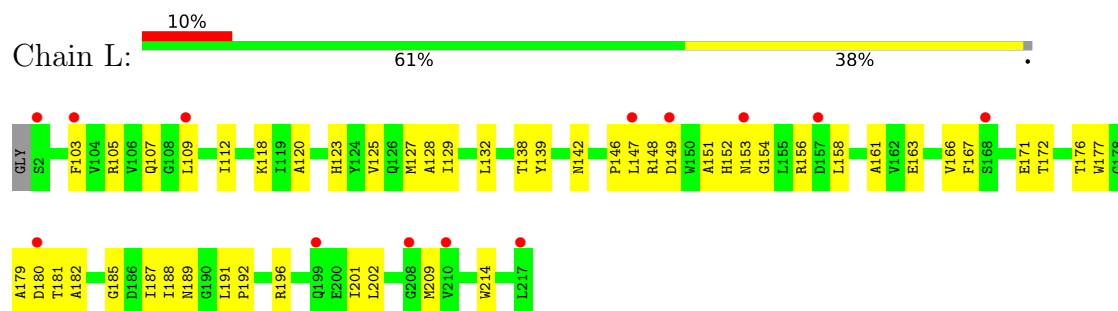
- Molecule 1: Protease NS2-3 (p23)



- Molecule 1: Protease NS2-3 (p23)



- Molecule 1: Protease NS2-3 (p23)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	109.81Å 68.82Å 125.16Å 90.00° 105.88° 90.00°	Depositor
Resolution (Å)	30.00 – 2.28 30.00 – 2.28	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.28) 98.2 (30.00-2.28)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.93 (at 2.29Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.226 , 0.268 0.236 , 0.280	Depositor DCC
R_{free} test set	8206 reflections (10.04%)	wwPDB-VP
Wilson B-factor (Å ²)	28.9	Xtriage
Anisotropy	0.445	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11930	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.13 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.4826e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BOG, DMU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.45	0/994	0.95	7/1347 (0.5%)
1	B	0.42	0/978	0.94	2/1329 (0.2%)
1	C	0.51	0/986	0.93	2/1338 (0.1%)
1	D	0.40	0/978	0.89	1/1327 (0.1%)
1	E	0.48	0/984	0.97	8/1335 (0.6%)
1	F	0.45	0/970	0.93	4/1320 (0.3%)
1	G	0.49	0/971	0.97	5/1320 (0.4%)
1	H	0.44	0/978	0.92	3/1328 (0.2%)
1	I	0.44	0/972	0.91	3/1322 (0.2%)
1	J	0.42	0/990	0.90	0/1343
1	K	0.45	0/968	0.95	4/1317 (0.3%)
1	L	0.38	0/972	0.89	2/1321 (0.2%)
All	All	0.45	0/11741	0.93	41/15947 (0.3%)

There are no bond length outliers.

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	GLY	N-CA-C	-7.80	104.54	114.37
1	F	185	GLY	N-CA-C	-7.53	105.51	114.48
1	G	185	GLY	N-CA-C	-7.51	105.54	113.58
1	B	152	HIS	N-CA-C	-7.06	101.21	110.53
1	H	2	SER	N-CA-C	-6.42	103.79	111.69
1	A	145	THR	CA-C-N	6.31	126.34	119.90
1	A	145	THR	C-N-CA	6.31	126.34	119.90
1	I	203	LEU	N-CA-C	6.31	121.14	113.38
1	F	160	VAL	N-CA-C	-6.22	106.64	113.43
1	B	185	GLY	N-CA-C	-6.10	106.66	113.79
1	L	185	GLY	N-CA-C	-5.94	106.84	113.79
1	D	185	GLY	N-CA-C	-5.89	106.95	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	111	ARG	N-CA-C	-5.88	104.95	111.36
1	L	151	ALA	N-CA-C	5.78	118.21	110.35
1	I	152	HIS	N-CA-C	-5.76	102.38	110.50
1	G	152	HIS	N-CA-C	-5.66	102.03	110.23
1	K	145	THR	CA-C-N	5.64	126.89	119.84
1	K	145	THR	C-N-CA	5.64	126.89	119.84
1	C	132	LEU	N-CA-C	-5.62	105.23	111.36
1	C	185	GLY	N-CA-C	-5.46	107.48	114.37
1	K	185	GLY	N-CA-C	-5.41	107.55	114.37
1	H	151	ALA	N-CA-C	5.40	117.30	110.33
1	G	145	THR	CA-C-N	5.31	125.61	119.93
1	G	145	THR	C-N-CA	5.31	125.61	119.93
1	E	145	THR	CA-C-N	5.28	126.44	119.84
1	E	145	THR	C-N-CA	5.28	126.44	119.84
1	E	126	GLN	N-CA-C	-5.28	105.61	111.36
1	E	191	LEU	CA-C-N	5.26	125.18	119.76
1	E	191	LEU	C-N-CA	5.26	125.18	119.76
1	F	145	THR	CA-C-N	5.24	126.39	119.84
1	F	145	THR	C-N-CA	5.24	126.39	119.84
1	A	152	HIS	N-CA-C	-5.24	103.12	110.50
1	A	160	VAL	N-CA-C	-5.20	106.83	113.22
1	H	185	GLY	N-CA-C	-5.19	107.72	113.79
1	E	185	GLY	N-CA-C	-5.12	107.92	114.37
1	K	153	ASN	N-CA-C	5.12	117.52	111.33
1	A	175	ILE	N-CA-C	5.07	116.66	108.85
1	G	151	ALA	N-CA-C	5.07	118.20	110.20
1	E	117	ARG	N-CA-C	5.04	117.50	111.71
1	A	153	ASN	N-CA-C	5.04	118.20	111.75
1	E	151	ALA	N-CA-C	5.03	118.15	110.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	974	0	1012	43	0
1	B	958	0	979	42	0
1	C	966	0	995	36	0
1	D	958	0	989	32	0
1	E	964	0	997	36	0
1	F	950	0	962	38	0
1	G	951	0	971	35	0
1	H	958	0	984	38	0
1	I	952	0	968	29	0
1	J	970	0	1001	33	0
1	K	948	0	964	53	0
1	L	952	0	973	47	0
2	A	60	0	84	4	0
2	B	20	0	28	1	0
2	C	20	0	28	1	0
2	F	40	0	56	0	0
2	H	20	0	28	4	0
2	I	20	0	28	0	0
2	J	20	0	28	0	0
2	K	20	0	28	0	0
3	I	33	0	37	0	0
4	A	16	0	0	0	0
4	B	10	0	0	0	0
4	C	24	0	0	2	0
4	D	14	0	0	0	0
4	E	29	0	0	1	0
4	F	13	0	0	0	0
4	G	15	0	0	1	0
4	H	13	0	0	0	0
4	I	14	0	0	0	0
4	J	8	0	0	0	0
4	K	13	0	0	0	0
4	L	7	0	0	0	0
All	All	11930	0	12140	377	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (377) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:179:ALA:HA	1:L:201:ILE:HD11	1.30	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:179:ALA:HA	1:H:201:ILE:HD11	1.23	1.10
1:G:179:ALA:HA	1:G:201:ILE:HD11	1.40	1.02
1:D:111:ARG:HH11	1:D:111:ARG:HA	1.26	0.99
1:F:179:ALA:HA	1:F:201:ILE:HD11	1.43	0.96
1:B:196:ARG:HD3	1:B:215:ARG:HH12	1.31	0.95
1:C:127:MET:HE3	1:C:158:LEU:HD13	1.50	0.93
1:K:179:ALA:HA	1:K:201:ILE:HD11	1.51	0.92
1:A:105:ARG:HH11	1:A:138:THR:HG22	1.36	0.91
1:A:174:LEU:HD11	1:B:200:GLU:HB3	1.52	0.90
1:E:172:THR:HG23	1:F:202:LEU:HD11	1.54	0.90
1:C:127:MET:HE2	1:C:167:PHE:CD2	2.06	0.90
1:H:127:MET:HE3	1:H:158:LEU:HB3	1.53	0.89
1:G:152:HIS:HD2	1:G:154:GLY:H	1.22	0.88
1:B:156:ARG:HG3	1:B:156:ARG:HH11	1.38	0.86
1:E:152:HIS:HD2	1:E:154:GLY:H	1.24	0.86
1:J:110:LEU:CD1	1:J:145:THR:HG21	2.05	0.86
1:D:111:ARG:HA	1:D:111:ARG:NH1	1.90	0.85
1:A:152:HIS:HD2	1:A:154:GLY:H	1.26	0.84
1:G:148:ARG:HH11	1:G:148:ARG:HG3	1.43	0.83
1:H:152:HIS:HD2	1:H:154:GLY:H	1.26	0.81
1:B:152:HIS:HD2	1:B:154:GLY:H	1.28	0.81
1:E:112:ILE:HG22	1:E:129:ILE:HD13	1.64	0.80
1:F:127:MET:HE3	1:F:158:LEU:HB3	1.62	0.80
1:A:133:GLY:O	1:A:136:THR:HG22	1.82	0.79
1:F:127:MET:HE2	1:F:167:PHE:CD2	2.18	0.79
1:L:142:ASN:ND2	1:L:146:PRO:HA	1.99	0.78
1:B:127:MET:HE3	1:B:158:LEU:HB3	1.65	0.78
1:D:179:ALA:HA	1:D:201:ILE:HD11	1.65	0.77
1:E:152:HIS:CD2	1:E:154:GLY:H	2.03	0.77
1:E:179:ALA:HA	1:E:201:ILE:HD11	1.65	0.76
1:H:179:ALA:HA	1:H:201:ILE:CD1	2.12	0.76
1:I:152:HIS:HD2	1:I:154:GLY:H	1.31	0.76
1:G:152:HIS:CD2	1:G:154:GLY:H	2.05	0.74
1:E:194:SER:HB3	1:E:206:ALA:HB2	1.68	0.74
1:K:117:ARG:HD3	1:K:118:LYS:NZ	2.03	0.73
1:C:204:GLY:HA3	1:D:172:THR:HA	1.71	0.73
1:K:4:MET:HE1	1:K:188:ILE:HD11	1.69	0.73
1:F:112:ILE:HG22	1:F:129:ILE:HD13	1.71	0.73
1:I:112:ILE:HG22	1:I:129:ILE:HD13	1.70	0.72
1:K:4:MET:SD	1:K:188:ILE:HD11	2.30	0.72
1:B:142:ASN:HD22	1:B:147:LEU:HG	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:ALA:HA	1:A:201:ILE:HD11	1.72	0.71
1:I:209:MET:HG3	1:I:214:TRP:CD1	2.25	0.71
1:K:174:LEU:HD11	1:L:214:TRP:HH2	1.54	0.71
1:B:142:ASN:ND2	1:B:147:LEU:HG	2.05	0.71
1:B:127:MET:CE	1:B:158:LEU:HB3	2.21	0.70
1:E:172:THR:CG2	1:F:202:LEU:HD11	2.21	0.70
1:L:142:ASN:HD22	1:L:146:PRO:HA	1.57	0.70
1:A:174:LEU:CD1	1:B:200:GLU:HB3	2.22	0.70
1:D:171:GLU:CD	1:D:173:LYS:HE3	2.17	0.70
1:A:105:ARG:NH1	1:A:138:THR:HG22	2.07	0.69
1:B:127:MET:HE2	1:B:167:PHE:CD2	2.27	0.69
1:I:152:HIS:CD2	1:I:154:GLY:H	2.11	0.69
1:A:131:LYS:O	1:A:135:LEU:HD23	1.94	0.68
1:J:112:ILE:HG22	1:J:129:ILE:HD13	1.76	0.67
1:D:147:LEU:HD23	1:D:150:TRP:CZ2	2.30	0.67
1:K:127:MET:HE2	1:K:167:PHE:CD2	2.30	0.67
1:E:189:ASN:H	1:F:189:ASN:ND2	1.93	0.67
1:B:196:ARG:HD3	1:B:215:ARG:NH1	2.07	0.66
1:C:112:ILE:HG22	1:C:129:ILE:HD13	1.78	0.66
1:K:192:PRO:O	1:K:203:LEU:O	2.14	0.66
1:A:105:ARG:HH11	1:A:138:THR:CG2	2.06	0.66
1:I:189:ASN:ND2	1:J:189:ASN:H	1.92	0.66
1:I:4:MET:HE2	1:J:177:TRP:CG	2.32	0.65
1:A:136:THR:CG2	1:A:138:THR:HG23	2.27	0.65
1:G:99:LYS:O	1:G:99:LYS:HG2	1.97	0.64
1:J:110:LEU:HD13	1:J:145:THR:HG21	1.80	0.64
1:G:140:VAL:HG12	4:G:221:HOH:O	1.96	0.64
1:K:4:MET:CE	1:K:188:ILE:HD11	2.27	0.64
1:B:156:ARG:HG3	1:B:156:ARG:NH1	2.13	0.63
1:B:142:ASN:ND2	1:B:147:LEU:H	1.97	0.63
1:A:152:HIS:CD2	1:A:154:GLY:H	2.12	0.63
1:J:177:TRP:CZ2	1:J:188:ILE:HD11	2.34	0.63
1:C:192:PRO:O	1:C:203:LEU:O	2.17	0.62
1:E:189:ASN:ND2	1:F:189:ASN:H	1.97	0.62
1:J:177:TRP:CH2	1:J:201:ILE:HD13	2.35	0.62
1:C:122:GLY:O	1:C:125:VAL:HG13	1.99	0.62
1:E:189:ASN:H	1:F:189:ASN:HD21	1.47	0.62
1:I:189:ASN:H	1:J:189:ASN:ND2	1.97	0.62
1:E:189:ASN:HD21	1:F:189:ASN:H	1.46	0.61
1:I:194:SER:HB3	1:I:206:ALA:HB2	1.82	0.61
1:E:161:ALA:HB1	1:F:207:ASP:OD2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:148:ARG:HG3	1:G:148:ARG:NH1	2.15	0.61
1:A:142:ASN:ND2	1:A:146:PRO:HA	2.15	0.61
1:H:174:LEU:N	1:H:174:LEU:HD12	2.16	0.61
1:C:189:ASN:H	1:D:189:ASN:ND2	1.99	0.61
1:G:112:ILE:HG22	1:G:129:ILE:HD13	1.82	0.61
1:H:105:ARG:HH11	1:H:138:THR:HB	1.67	0.60
1:J:177:TRP:HH2	1:J:201:ILE:HD13	1.67	0.60
1:C:127:MET:CE	1:C:158:LEU:HD13	2.29	0.60
1:F:147:LEU:HD22	1:F:150:TRP:CZ2	2.37	0.60
1:F:122:GLY:O	1:F:125:VAL:HG22	2.02	0.60
1:B:177:TRP:CZ2	1:B:188:ILE:HD11	2.37	0.59
1:H:192:PRO:O	1:H:203:LEU:O	2.20	0.59
1:I:189:ASN:HD21	1:J:189:ASN:H	1.51	0.59
1:D:119:ILE:HG22	1:D:122:GLY:CA	2.32	0.59
1:E:104:VAL:HA	1:E:107:GLN:HE21	1.68	0.59
1:A:174:LEU:HD13	1:B:214:TRP:HH2	1.67	0.59
1:F:127:MET:CE	1:F:158:LEU:HB3	2.32	0.58
1:E:123:HIS:H	1:E:123:HIS:CD2	2.20	0.58
1:K:172:THR:CG2	1:L:202:LEU:HD11	2.33	0.58
1:L:127:MET:HE3	1:L:158:LEU:HB3	1.86	0.58
1:H:105:ARG:NH1	1:H:138:THR:HB	2.19	0.58
1:K:127:MET:HE3	1:K:158:LEU:HB3	1.83	0.58
1:L:128:ALA:O	1:L:132:LEU:HD13	2.04	0.57
1:A:136:THR:HG23	1:A:138:THR:HG23	1.85	0.57
1:C:174:LEU:CD2	1:D:200:GLU:HB3	2.34	0.57
1:D:119:ILE:HG22	1:D:122:GLY:HA3	1.85	0.57
1:A:169:ARG:CZ	1:F:169:ARG:HE	2.16	0.57
1:I:199:GLN:HA	1:I:199:GLN:OE1	2.03	0.57
1:K:209:MET:HE3	1:K:214:TRP:NE1	2.20	0.57
1:E:139:TYR:CE1	1:F:192:PRO:HG3	2.40	0.56
1:J:147:LEU:HD22	1:J:150:TRP:CZ2	2.40	0.56
1:E:202:LEU:HD11	1:F:172:THR:CG2	2.35	0.56
1:G:170:MET:HE3	1:H:205:PRO:HG3	1.88	0.56
1:I:174:LEU:HD22	1:J:214:TRP:CH2	2.39	0.56
1:I:175:ILE:HD11	1:J:201:ILE:HD11	1.87	0.56
1:K:142:ASN:ND2	1:K:147:LEU:H	2.03	0.56
1:E:179:ALA:CA	1:E:201:ILE:HD11	2.33	0.56
1:F:116:ALA:HB1	1:F:125:VAL:HG21	1.88	0.56
1:K:112:ILE:HG22	1:K:129:ILE:HD13	1.87	0.56
1:A:181:THR:CG2	1:J:148:ARG:HD2	2.36	0.56
1:H:152:HIS:CD2	1:H:154:GLY:H	2.17	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:TRP:CZ2	1:A:188:ILE:HD11	2.41	0.55
1:C:139:TYR:CE1	1:D:192:PRO:HG3	2.42	0.55
1:K:209:MET:O	1:K:214:TRP:HD1	1.88	0.55
1:A:189:ASN:ND2	1:B:189:ASN:H	2.04	0.55
1:L:179:ALA:HA	1:L:201:ILE:CD1	2.21	0.55
1:G:182:ALA:HB2	1:G:201:ILE:HD13	1.88	0.55
1:B:126:GLN:HE22	1:B:152:HIS:H	1.55	0.55
2:A:218:BOG:H3'2	1:E:104:VAL:HG12	1.89	0.55
1:H:107:GLN:O	1:H:111:ARG:HG3	2.06	0.55
1:I:202:LEU:HD12	1:J:174:LEU:HD23	1.89	0.55
1:C:202:LEU:HG	1:C:214:TRP:CZ3	2.41	0.54
1:H:196:ARG:HG2	1:H:197:ARG:N	2.21	0.54
1:K:117:ARG:HD3	1:K:118:LYS:HZ2	1.70	0.54
1:D:155:LEU:HD13	1:D:155:LEU:C	2.33	0.54
1:J:171:GLU:OE2	1:J:173:LYS:HE3	2.07	0.54
1:A:181:THR:HG22	1:J:148:ARG:HD2	1.90	0.54
1:E:107:GLN:O	1:E:111:ARG:HG3	2.08	0.54
1:J:177:TRP:HH2	1:J:201:ILE:CD1	2.21	0.54
1:K:147:LEU:HD22	1:K:150:TRP:CZ2	2.43	0.54
1:L:209:MET:HG2	1:L:214:TRP:CD1	2.43	0.54
1:G:147:LEU:HD22	1:G:150:TRP:CZ2	2.44	0.53
1:K:172:THR:HG22	1:L:202:LEU:HD11	1.90	0.53
1:I:180:ASP:OD1	1:I:196:ARG:NH2	2.41	0.53
1:G:203:LEU:HD11	1:H:175:ILE:HD13	1.90	0.53
1:H:104:VAL:HG12	2:H:218:BOG:H3'2	1.90	0.53
1:L:152:HIS:HD2	1:L:154:GLY:H	1.55	0.53
1:A:147:LEU:HD22	1:A:150:TRP:CZ2	2.44	0.53
1:C:127:MET:HE2	1:C:167:PHE:HD2	1.66	0.52
1:C:143:HIS:ND1	1:C:163:GLU:OE1	2.41	0.52
1:K:117:ARG:HD3	1:K:118:LYS:HZ1	1.73	0.52
1:K:202:LEU:HD11	1:L:172:THR:HG22	1.92	0.52
1:K:209:MET:HB3	1:K:214:TRP:CD1	2.44	0.52
1:J:115:LEU:O	1:J:115:LEU:HD23	2.10	0.52
1:C:104:VAL:HG13	2:C:218:BOG:H1'1	1.91	0.52
1:K:139:TYR:CE1	1:L:192:PRO:HG3	2.45	0.52
1:F:182:ALA:HB2	1:F:201:ILE:HD13	1.90	0.52
1:K:189:ASN:ND2	1:L:189:ASN:H	2.07	0.52
1:A:200:GLU:HG2	1:B:176:THR:HG22	1.91	0.52
1:C:127:MET:CE	1:C:158:LEU:HB3	2.40	0.52
1:I:103:PHE:O	1:I:107:GLN:HG2	2.09	0.52
1:C:142:ASN:ND2	1:C:146:PRO:HA	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:132:LEU:O	1:K:136:THR:HG23	2.10	0.51
1:L:180:ASP:HA	1:L:196:ARG:NH1	2.25	0.51
1:A:169:ARG:HD3	1:F:169:ARG:HH21	1.73	0.51
1:F:209:MET:HE2	1:F:212:LYS:HD2	1.91	0.51
1:K:105:ARG:NH2	1:K:137:GLY:O	2.43	0.51
1:B:152:HIS:CD2	1:B:154:GLY:H	2.18	0.51
1:C:122:GLY:HA2	1:C:125:VAL:CG1	2.40	0.51
1:A:142:ASN:HD22	1:A:146:PRO:HA	1.74	0.51
2:A:220:BOG:H5'1	1:E:98:LEU:HD11	1.92	0.51
1:D:142:ASN:OD1	1:D:146:PRO:HA	2.11	0.51
1:K:142:ASN:HD22	1:K:147:LEU:H	1.59	0.51
1:C:197:ARG:NH2	1:C:214:TRP:HE1	2.09	0.51
1:G:142:ASN:ND2	1:G:147:LEU:H	2.09	0.51
1:I:202:LEU:HD11	1:J:172:THR:CG2	2.40	0.50
1:I:214:TRP:CH2	1:J:174:LEU:HD22	2.46	0.50
1:D:171:GLU:OE2	1:D:173:LYS:HE3	2.10	0.50
1:I:139:TYR:CE1	1:J:192:PRO:HG3	2.46	0.50
1:L:142:ASN:ND2	1:L:147:LEU:H	2.08	0.50
1:K:196:ARG:HB2	1:K:217:LEU:HD21	1.93	0.50
1:B:161:ALA:HB3	1:B:166:VAL:HG22	1.93	0.50
1:G:171:GLU:OE1	1:G:173:LYS:NZ	2.45	0.50
1:K:202:LEU:HD11	1:L:172:THR:CG2	2.42	0.50
1:I:189:ASN:H	1:J:189:ASN:HD21	1.58	0.50
1:D:107:GLN:O	1:D:111:ARG:HG2	2.12	0.50
1:A:189:ASN:HD21	1:B:189:ASN:H	1.60	0.49
1:B:104:VAL:CG1	2:B:218:BOG:H1'2	2.42	0.49
1:K:127:MET:HE2	1:K:167:PHE:CG	2.48	0.49
1:A:174:LEU:HD11	1:B:200:GLU:CB	2.35	0.49
1:K:174:LEU:CD1	1:L:214:TRP:HH2	2.24	0.49
1:J:201:ILE:O	1:J:201:ILE:HG13	2.11	0.49
1:H:130:ILE:HD11	1:H:150:TRP:CH2	2.48	0.49
1:J:119:ILE:HG23	1:J:122:GLY:CA	2.42	0.49
1:L:103:PHE:O	1:L:107:GLN:HG3	2.13	0.49
1:D:127:MET:O	1:D:131:LYS:HG3	2.11	0.49
1:A:174:LEU:HD13	1:B:214:TRP:CH2	2.48	0.49
1:A:188:ILE:HD12	1:A:203:LEU:HD21	1.95	0.49
1:G:189:ASN:ND2	1:H:189:ASN:H	2.10	0.49
2:A:218:BOG:O5	1:E:111:ARG:HD2	2.13	0.48
1:E:192:PRO:HG3	1:F:139:TYR:CE1	2.48	0.48
1:B:156:ARG:HH11	1:B:156:ARG:CG	2.18	0.48
1:K:127:MET:CE	1:K:158:LEU:HB3	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:166:VAL:HG11	1:G:170:MET:HE2	1.95	0.48
1:K:95:ALA:HB3	1:L:187:ILE:HB	1.94	0.48
1:B:108:GLY:O	1:B:112:ILE:HG13	2.14	0.48
1:D:122:GLY:O	1:D:126:GLN:HG3	2.14	0.48
1:H:174:LEU:N	1:H:174:LEU:CD1	2.76	0.48
1:I:112:ILE:CG2	1:I:129:ILE:HD13	2.43	0.48
1:L:103:PHE:H	1:L:103:PHE:HD1	1.61	0.48
1:C:174:LEU:HD21	1:D:200:GLU:HB3	1.94	0.48
1:L:148:ARG:HG3	1:L:149:ASP:OD1	2.13	0.48
1:A:200:GLU:HG2	1:B:176:THR:CG2	2.44	0.48
1:C:189:ASN:H	1:D:189:ASN:HD21	1.62	0.48
1:J:97:LEU:HD22	1:J:136:THR:HA	1.96	0.48
1:A:142:ASN:ND2	1:A:147:LEU:H	2.11	0.47
1:I:196:ARG:HG2	1:I:197:ARG:N	2.28	0.47
1:K:204:GLY:HA3	1:L:171:GLU:O	2.14	0.47
1:E:147:LEU:HD22	1:E:150:TRP:CZ2	2.49	0.47
1:F:116:ALA:CB	1:F:125:VAL:HG21	2.44	0.47
1:H:111:ARG:CZ	2:H:218:BOG:H5	2.44	0.47
1:C:187:ILE:HB	1:D:95:ALA:HB3	1.96	0.47
2:H:218:BOG:H4	1:L:120:ALA:HB3	1.96	0.47
1:A:215:ARG:O	1:A:215:ARG:HG3	2.13	0.47
1:C:142:ASN:HD22	1:C:146:PRO:HA	1.79	0.47
1:I:171:GLU:OE1	1:I:173:LYS:HE3	2.13	0.47
1:L:147:LEU:HD12	1:L:156:ARG:HD3	1.96	0.47
1:C:4:MET:HE3	1:D:188:ILE:HD12	1.96	0.47
1:K:4:MET:HE2	1:L:177:TRP:CG	2.50	0.47
1:K:202:LEU:HD23	1:K:206:ALA:HB2	1.97	0.47
1:D:132:LEU:HD23	1:D:135:LEU:HD12	1.96	0.47
1:G:192:PRO:HG3	1:H:139:TYR:CE1	2.50	0.47
1:K:111:ARG:HG2	1:K:111:ARG:HH11	1.79	0.47
1:D:161:ALA:HB3	1:D:166:VAL:HG22	1.96	0.47
1:G:103:PHE:CD2	1:G:103:PHE:N	2.70	0.47
1:I:217:LEU:O	1:J:143:HIS:NE2	2.37	0.47
1:K:192:PRO:HG3	1:L:139:TYR:CE1	2.50	0.47
1:B:127:MET:HG3	1:B:167:PHE:CD2	2.51	0.46
1:J:161:ALA:O	1:J:165:VAL:HA	2.15	0.46
1:B:156:ARG:NH1	1:B:156:ARG:CG	2.78	0.46
1:E:123:HIS:HE1	4:E:237:HOH:O	1.98	0.46
1:C:180:ASP:OD1	1:C:196:ARG:NH2	2.47	0.46
1:G:4:MET:HE2	1:H:177:TRP:CG	2.50	0.46
1:G:170:MET:CE	1:H:205:PRO:HG3	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:194:SER:HB3	1:G:206:ALA:HB2	1.96	0.46
1:H:127:MET:HE2	1:H:167:PHE:CD2	2.50	0.46
1:A:172:THR:HG23	1:B:202:LEU:HD22	1.97	0.46
1:G:142:ASN:HD22	1:G:147:LEU:H	1.63	0.46
1:L:127:MET:CE	1:L:158:LEU:HB3	2.45	0.46
1:A:112:ILE:HG22	1:A:129:ILE:HD13	1.98	0.46
1:H:127:MET:HG3	1:H:167:PHE:CD2	2.51	0.46
1:K:4:MET:HE3	1:L:188:ILE:HD11	1.97	0.46
1:K:142:ASN:HB3	1:K:163:GLU:OE2	2.16	0.46
1:K:196:ARG:CB	1:K:217:LEU:HD21	2.45	0.46
1:C:202:LEU:HD11	1:C:209:MET:HE2	1.98	0.46
1:H:143:HIS:ND1	1:H:163:GLU:OE1	2.43	0.46
1:K:193:VAL:CG1	1:K:217:LEU:HD12	2.46	0.46
1:F:209:MET:HA	1:F:209:MET:HE3	1.98	0.45
1:H:130:ILE:HD11	1:H:150:TRP:HH2	1.80	0.45
1:H:111:ARG:NH2	2:H:218:BOG:H5	2.31	0.45
1:A:142:ASN:HB3	1:A:163:GLU:OE2	2.16	0.45
1:F:122:GLY:O	1:F:126:GLN:HG3	2.17	0.45
1:G:172:THR:HA	1:H:204:GLY:HA3	1.98	0.45
1:K:4:MET:HE3	1:L:188:ILE:CD1	2.46	0.45
1:B:147:LEU:HD11	1:B:162:VAL:HG11	1.98	0.45
1:E:112:ILE:HG22	1:E:129:ILE:CD1	2.42	0.45
1:J:142:ASN:HB3	1:J:163:GLU:OE2	2.16	0.45
1:C:156:ARG:HB3	4:C:231:HOH:O	2.15	0.45
1:A:163:GLU:HB2	1:B:207:ASP:OD2	2.17	0.45
1:F:127:MET:CE	1:F:167:PHE:CD2	2.95	0.45
1:D:143:HIS:ND1	1:D:163:GLU:OE1	2.45	0.45
1:K:199:GLN:O	1:L:176:THR:HG23	2.16	0.45
1:L:161:ALA:HB3	1:L:166:VAL:HG22	1.98	0.45
1:L:187:ILE:O	1:L:188:ILE:HD13	2.16	0.45
1:G:148:ARG:O	1:G:148:ARG:HG2	2.15	0.45
1:K:181:THR:O	1:K:181:THR:HG22	2.17	0.45
1:E:179:ALA:HA	1:E:201:ILE:CD1	2.42	0.44
1:E:182:ALA:O	1:E:217:LEU:HD13	2.17	0.44
1:G:176:THR:O	1:G:176:THR:HG22	2.16	0.44
1:A:160:VAL:HG12	1:A:160:VAL:O	2.17	0.44
1:F:161:ALA:O	1:F:165:VAL:HA	2.17	0.44
1:H:182:ALA:CB	1:H:201:ILE:HD13	2.47	0.44
1:I:117:ARG:NH2	1:I:148:ARG:O	2.51	0.44
1:F:147:LEU:HB3	1:F:151:ALA:CB	2.47	0.44
1:F:174:LEU:N	1:F:174:LEU:HD12	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:127:MET:HE2	1:H:167:PHE:HB3	2.00	0.44
1:I:191:LEU:HB3	1:I:203:LEU:O	2.17	0.44
1:C:162:VAL:HA	1:C:165:VAL:HA	2.00	0.44
1:E:105:ARG:NH2	1:E:137:GLY:O	2.51	0.44
1:L:182:ALA:HB2	1:L:201:ILE:HD13	1.98	0.44
1:K:202:LEU:HD23	1:K:206:ALA:CB	2.48	0.44
1:F:191:LEU:HA	1:F:192:PRO:HD3	1.90	0.44
1:G:182:ALA:CB	1:G:201:ILE:HD13	2.47	0.44
1:B:197:ARG:HH11	1:B:214:TRP:NE1	2.14	0.44
1:K:174:LEU:CD1	1:L:214:TRP:CH2	3.01	0.44
1:L:191:LEU:HA	1:L:192:PRO:HD3	1.82	0.44
1:A:177:TRP:CH2	1:A:188:ILE:HD11	2.52	0.43
1:K:161:ALA:O	1:K:165:VAL:HA	2.18	0.43
1:L:152:HIS:CD2	1:L:154:GLY:H	2.35	0.43
1:L:125:VAL:O	1:L:129:ILE:HG13	2.19	0.43
1:B:112:ILE:HG22	1:B:129:ILE:HD13	2.00	0.43
1:G:99:LYS:O	1:G:99:LYS:CG	2.66	0.43
1:A:161:ALA:O	1:A:165:VAL:HA	2.18	0.43
1:A:202:LEU:HD11	1:B:172:THR:CG2	2.49	0.43
1:E:118:LYS:HE2	1:E:118:LYS:HA	2.00	0.43
1:A:191:LEU:HA	1:A:192:PRO:HD3	1.85	0.43
1:C:171:GLU:HG2	1:C:173:LYS:HG3	2.01	0.43
1:C:202:LEU:HD23	1:C:202:LEU:HA	1.89	0.43
1:D:110:LEU:HD22	1:D:150:TRP:CD2	2.54	0.43
1:E:123:HIS:H	1:E:123:HIS:HD2	1.62	0.43
1:J:116:ALA:O	1:J:119:ILE:HG22	2.18	0.43
1:K:142:ASN:HB2	1:K:162:VAL:HB	2.01	0.43
1:K:207:ASP:OD1	1:L:163:GLU:HB2	2.19	0.43
1:B:197:ARG:HD3	1:B:214:TRP:CE2	2.53	0.43
1:F:127:MET:HE2	1:F:167:PHE:CG	2.53	0.43
1:F:143:HIS:ND1	1:F:163:GLU:OE1	2.50	0.43
1:A:174:LEU:CD1	1:B:214:TRP:HH2	2.32	0.43
1:B:127:MET:HE3	1:B:158:LEU:CB	2.43	0.42
1:E:123:HIS:CD2	1:E:123:HIS:N	2.87	0.42
1:F:182:ALA:HB2	1:F:201:ILE:CD1	2.49	0.42
1:K:204:GLY:HA3	1:L:172:THR:HA	2.01	0.42
1:L:112:ILE:HG22	1:L:129:ILE:HD13	2.01	0.42
1:B:161:ALA:O	1:B:165:VAL:HA	2.18	0.42
1:G:170:MET:HE3	1:H:205:PRO:HD3	2.01	0.42
1:H:127:MET:HG3	1:H:167:PHE:CE2	2.54	0.42
1:H:196:ARG:CG	1:H:197:ARG:N	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:147:LEU:HD22	1:I:150:TRP:CZ2	2.54	0.42
1:I:148:ARG:NH1	1:I:149:ASP:OD2	2.52	0.42
1:G:123:HIS:HB3	1:G:152:HIS:CD2	2.55	0.42
1:L:105:ARG:HD2	1:L:138:THR:OG1	2.19	0.42
1:B:171:GLU:CD	1:B:173:LYS:HE3	2.44	0.42
1:F:155:LEU:C	1:F:155:LEU:HD13	2.45	0.42
1:K:174:LEU:HD11	1:L:214:TRP:CH2	2.43	0.42
1:G:187:ILE:HB	1:H:95:ALA:HB3	2.01	0.42
1:G:142:ASN:ND2	1:G:146:PRO:HA	2.34	0.42
1:D:161:ALA:O	1:D:165:VAL:HA	2.20	0.42
1:C:202:LEU:CD2	1:D:174:LEU:HD23	2.50	0.42
1:J:119:ILE:HG12	1:J:120:ALA:N	2.35	0.42
1:C:155:LEU:HD13	1:C:155:LEU:O	2.19	0.42
1:E:4:MET:HE2	1:F:177:TRP:CG	2.55	0.42
1:K:193:VAL:HG12	1:K:217:LEU:HD12	2.02	0.42
1:E:112:ILE:CG2	1:E:129:ILE:HD13	2.44	0.41
1:F:161:ALA:HB3	1:F:166:VAL:HG22	2.01	0.41
1:G:117:ARG:NH2	1:G:148:ARG:O	2.53	0.41
1:L:127:MET:HE2	1:L:167:PHE:CD2	2.55	0.41
1:A:104:VAL:CG1	2:A:219:BOG:H1'1	2.49	0.41
1:L:123:HIS:HB3	1:L:152:HIS:CD2	2.55	0.41
1:I:192:PRO:O	1:I:203:LEU:O	2.38	0.41
1:E:205:PRO:HA	1:F:163:GLU:O	2.20	0.41
1:L:181:THR:O	1:L:181:THR:HG22	2.20	0.41
1:C:163:GLU:O	1:D:205:PRO:HA	2.19	0.41
1:G:179:ALA:HA	1:G:201:ILE:CD1	2.28	0.41
1:G:189:ASN:HD21	1:H:189:ASN:H	1.68	0.41
1:K:189:ASN:HD21	1:L:189:ASN:H	1.68	0.41
1:J:110:LEU:HD12	1:J:145:THR:HG21	1.99	0.41
1:A:172:THR:HG23	1:B:202:LEU:CD2	2.51	0.41
1:B:141:TYR:HB3	1:B:163:GLU:OE1	2.21	0.41
1:C:207:ASP:OD2	1:D:161:ALA:HB1	2.21	0.41
1:E:101:PRO:O	1:E:105:ARG:HG3	2.21	0.41
1:F:182:ALA:CB	1:F:201:ILE:HD13	2.50	0.41
1:H:127:MET:CE	1:H:167:PHE:CD2	3.04	0.41
1:D:191:LEU:HA	1:D:192:PRO:HD3	1.82	0.40
1:I:136:THR:O	1:I:136:THR:CG2	2.69	0.40
1:K:117:ARG:C	1:K:118:LYS:HD2	2.46	0.40
1:D:121:GLY:HA2	1:D:123:HIS:CE1	2.56	0.40
1:G:170:MET:HE3	1:H:205:PRO:CD	2.51	0.40
1:H:122:GLY:O	1:H:126:GLN:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:LEU:HD23	1:A:147:LEU:N	2.36	0.40
1:C:112:ILE:HG22	1:C:129:ILE:CD1	2.49	0.40
1:J:191:LEU:HA	1:J:192:PRO:HD3	1.74	0.40
1:E:152:HIS:HD2	1:E:154:GLY:N	2.04	0.40
1:H:155:LEU:O	1:H:158:LEU:N	2.55	0.40
1:C:95:ALA:HA	4:C:234:HOH:O	2.21	0.40
1:C:174:LEU:HD21	1:D:200:GLU:CD	2.46	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	125/128 (98%)	122 (98%)	3 (2%)	0	100	100
1	B	125/128 (98%)	120 (96%)	4 (3%)	1 (1%)	16	18
1	C	125/128 (98%)	122 (98%)	3 (2%)	0	100	100
1	D	125/128 (98%)	122 (98%)	2 (2%)	1 (1%)	16	18
1	E	125/128 (98%)	122 (98%)	3 (2%)	0	100	100
1	F	125/128 (98%)	123 (98%)	2 (2%)	0	100	100
1	G	125/128 (98%)	119 (95%)	6 (5%)	0	100	100
1	H	126/128 (98%)	116 (92%)	10 (8%)	0	100	100
1	I	125/128 (98%)	122 (98%)	3 (2%)	0	100	100
1	J	125/128 (98%)	122 (98%)	3 (2%)	0	100	100
1	K	125/128 (98%)	120 (96%)	5 (4%)	0	100	100
1	L	125/128 (98%)	117 (94%)	8 (6%)	0	100	100
All	All	1501/1536 (98%)	1447 (96%)	52 (4%)	2 (0%)	48	59

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	120	ALA
1	D	119	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	100/100 (100%)	92 (92%)	8 (8%)	11	13
1	B	97/100 (97%)	95 (98%)	2 (2%)	47	63
1	C	98/100 (98%)	91 (93%)	7 (7%)	13	17
1	D	96/100 (96%)	92 (96%)	4 (4%)	26	37
1	E	98/100 (98%)	89 (91%)	9 (9%)	8	10
1	F	95/100 (95%)	94 (99%)	1 (1%)	65	79
1	G	95/100 (95%)	89 (94%)	6 (6%)	16	21
1	H	96/100 (96%)	93 (97%)	3 (3%)	35	50
1	I	96/100 (96%)	91 (95%)	5 (5%)	21	28
1	J	99/100 (99%)	97 (98%)	2 (2%)	48	65
1	K	95/100 (95%)	89 (94%)	6 (6%)	16	21
1	L	96/100 (96%)	93 (97%)	3 (3%)	35	50
All	All	1161/1200 (97%)	1105 (95%)	56 (5%)	23	32

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	LEU
1	A	135	LEU
1	A	138	THR
1	A	140	VAL
1	A	147	LEU
1	A	155	LEU
1	A	171	GLU
1	A	212	LYS
1	B	156	ARG

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Mol	Chain	Res	Type
1	B	202	LEU
1	C	97	LEU
1	C	125	VAL
1	C	132	LEU
1	C	136	THR
1	C	140	VAL
1	C	147	LEU
1	C	174	LEU
1	D	111	ARG
1	D	119	ILE
1	D	202	LEU
1	D	203	LEU
1	E	123	HIS
1	E	125	VAL
1	E	135	LEU
1	E	136	THR
1	E	147	LEU
1	E	155	LEU
1	E	156	ARG
1	E	160	VAL
1	E	172	THR
1	F	209	MET
1	G	103	PHE
1	G	132	LEU
1	G	136	THR
1	G	147	LEU
1	G	164	PRO
1	G	174	LEU
1	H	94	GLN
1	H	138	THR
1	H	174	LEU
1	I	94	GLN
1	I	140	VAL
1	I	147	LEU
1	I	168	SER
1	I	199	GLN
1	J	147	LEU
1	J	175	ILE
1	K	111	ARG
1	K	125	VAL
1	K	147	LEU
1	K	171	GLU

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Mol	Chain	Res	Type
1	K	180	ASP
1	K	207	ASP
1	L	109	LEU
1	L	118	LYS
1	L	153	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	GLN
1	A	142	ASN
1	A	152	HIS
1	A	189	ASN
1	B	126	GLN
1	B	142	ASN
1	B	152	HIS
1	C	142	ASN
1	D	189	ASN
1	E	94	GLN
1	E	107	GLN
1	E	123	HIS
1	E	152	HIS
1	E	189	ASN
1	F	189	ASN
1	G	94	GLN
1	G	142	ASN
1	G	152	HIS
1	G	153	ASN
1	G	189	ASN
1	H	142	ASN
1	H	152	HIS
1	I	94	GLN
1	I	152	HIS
1	I	189	ASN
1	J	189	ASN
1	K	107	GLN
1	K	142	ASN
1	K	189	ASN
1	L	123	HIS
1	L	142	ASN
1	L	152	HIS
1	L	153	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	BOG	A	218	-	20,20,20	0.82	1 (5%)	25,25,25	0.64	0
2	BOG	H	218	-	20,20,20	1.11	1 (5%)	25,25,25	0.89	2 (8%)
2	BOG	B	218	-	20,20,20	0.83	2 (10%)	25,25,25	0.61	0
2	BOG	A	220	-	20,20,20	0.98	2 (10%)	25,25,25	1.45	2 (8%)
2	BOG	C	218	-	20,20,20	0.97	2 (10%)	25,25,25	0.65	0
2	BOG	F	218	-	20,20,20	0.91	2 (10%)	25,25,25	0.72	0
2	BOG	A	219	-	20,20,20	0.99	2 (10%)	25,25,25	0.64	0
2	BOG	K	218	-	20,20,20	0.89	1 (5%)	25,25,25	0.63	0
3	DMU	I	218	-	34,34,34	2.90	9 (26%)	45,45,45	4.29	20 (44%)
2	BOG	I	219	-	20,20,20	0.68	1 (5%)	25,25,25	0.66	0
2	BOG	J	218	-	20,20,20	0.75	0	25,25,25	0.61	0
2	BOG	F	219	-	20,20,20	0.85	1 (5%)	25,25,25	0.64	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BOG	A	218	-	-	6/11/31/31	0/1/1/1
2	BOG	H	218	-	-	2/11/31/31	0/1/1/1
2	BOG	B	218	-	-	2/11/31/31	0/1/1/1
2	BOG	A	220	-	-	5/11/31/31	0/1/1/1
2	BOG	C	218	-	-	4/11/31/31	0/1/1/1
2	BOG	F	218	-	-	5/11/31/31	0/1/1/1
2	BOG	A	219	-	-	5/11/31/31	0/1/1/1
2	BOG	K	218	-	-	6/11/31/31	0/1/1/1
3	DMU	I	218	-	5/5/10/10	10/19/59/59	0/2/2/2
2	BOG	I	219	-	-	6/11/31/31	0/1/1/1
2	BOG	J	218	-	-	3/11/31/31	0/1/1/1
2	BOG	F	219	-	-	6/11/31/31	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	218	DMU	O7-C3	-7.35	1.25	1.43
3	I	218	DMU	O16-C6	-6.55	1.29	1.40
3	I	218	DMU	O5-C4	-6.36	1.28	1.44
3	I	218	DMU	O7-C10	-5.82	1.25	1.41
3	I	218	DMU	O16-C18	-5.73	1.27	1.43
3	I	218	DMU	O1-C9	-5.72	1.30	1.44
2	H	218	BOG	O1-C1	3.74	1.46	1.40
3	I	218	DMU	O5-C6	-3.72	1.32	1.41
3	I	218	DMU	O1-C10	-3.38	1.33	1.41
2	A	219	BOG	O1-C1	3.05	1.45	1.40
2	A	220	BOG	O1-C1	3.03	1.45	1.40
2	C	218	BOG	O1-C1	2.85	1.44	1.40
3	I	218	DMU	C8-C9	2.58	1.58	1.53
2	F	219	BOG	O1-C1	2.57	1.44	1.40
2	K	218	BOG	O1-C1	2.54	1.44	1.40
2	F	218	BOG	O1-C1	2.38	1.44	1.40
2	C	218	BOG	O5-C1	2.36	1.47	1.41
2	A	218	BOG	O1-C1	2.26	1.44	1.40
2	B	218	BOG	O1-C1	2.17	1.43	1.40
2	A	219	BOG	O5-C1	2.10	1.47	1.41
2	A	220	BOG	O5-C1	2.09	1.47	1.41
2	I	219	BOG	O1-C1	2.06	1.43	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	218	BOG	O5-C1	2.04	1.47	1.41
2	F	218	BOG	O5-C1	2.03	1.47	1.41

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	218	DMU	C10-C5-C7	11.01	133.18	110.01
3	I	218	DMU	C1-C2-C3	10.36	133.20	109.68
3	I	218	DMU	C6-O5-C4	8.77	130.85	113.72
3	I	218	DMU	O1-C9-C8	7.96	124.05	109.70
3	I	218	DMU	O5-C4-C3	7.43	125.09	109.72
3	I	218	DMU	C7-C8-C9	6.88	122.72	110.23
3	I	218	DMU	C18-O16-C6	6.67	125.07	113.68
3	I	218	DMU	C8-C7-C5	-6.65	99.16	110.83
3	I	218	DMU	O5-C4-C57	6.65	122.92	106.44
3	I	218	DMU	O1-C9-C11	6.59	122.78	106.44
2	A	220	BOG	C1'-O1-C1	5.60	123.25	113.68
3	I	218	DMU	O5-C6-C1	5.28	121.22	110.37
3	I	218	DMU	O16-C6-C1	5.28	116.28	108.27
3	I	218	DMU	O5-C6-O16	5.27	122.49	110.04
3	I	218	DMU	C10-O1-C9	4.75	123.00	113.72
3	I	218	DMU	O7-C3-C2	3.94	117.25	107.23
3	I	218	DMU	O7-C10-C5	3.68	117.14	108.09
3	I	218	DMU	C2-C3-C4	-3.14	103.97	110.93
2	H	218	BOG	O1-C1-C2	2.99	112.82	108.27
3	I	218	DMU	C10-O7-C3	2.78	124.57	117.98
2	A	220	BOG	O1-C1-C2	2.69	112.35	108.27
3	I	218	DMU	O7-C3-C4	2.30	115.51	109.48
3	I	218	DMU	C6-C1-C2	-2.07	105.66	110.01
2	H	218	BOG	C1'-O1-C1	2.06	117.19	113.68

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	I	218	DMU	C2
3	I	218	DMU	C4
3	I	218	DMU	C6
3	I	218	DMU	C9
3	I	218	DMU	C5

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	218	BOG	C2-C1-O1-C1'
2	A	218	BOG	O5-C1-O1-C1'
2	A	220	BOG	O5-C1-O1-C1'
2	C	218	BOG	O5-C1-O1-C1'
2	F	219	BOG	O5-C1-O1-C1'
3	I	218	DMU	O5-C6-O16-C18
2	A	219	BOG	O5-C5-C6-O6
3	I	218	DMU	O6-C11-C9-O1
2	F	219	BOG	O5-C5-C6-O6
3	I	218	DMU	C3-C4-C57-O61
2	A	219	BOG	O5-C1-O1-C1'
2	F	218	BOG	O5-C1-O1-C1'
2	I	219	BOG	O5-C1-O1-C1'
2	K	218	BOG	O5-C1-O1-C1'
2	I	219	BOG	C3'-C4'-C5'-C6'
2	F	218	BOG	C4-C5-C6-O6
2	A	219	BOG	C4-C5-C6-O6
2	F	219	BOG	C4-C5-C6-O6
2	A	220	BOG	C2-C1-O1-C1'
2	F	218	BOG	C2-C1-O1-C1'
2	H	218	BOG	C2-C1-O1-C1'
2	I	219	BOG	C2-C1-O1-C1'
2	A	218	BOG	C4-C5-C6-O6
2	F	218	BOG	O5-C5-C6-O6
2	K	218	BOG	O5-C5-C6-O6
2	J	218	BOG	O1-C1'-C2'-C3'
2	B	218	BOG	O5-C1-O1-C1'
2	K	218	BOG	O1-C1'-C2'-C3'
2	A	218	BOG	O5-C5-C6-O6
2	A	219	BOG	O1-C1'-C2'-C3'
2	F	219	BOG	O1-C1'-C2'-C3'
2	B	218	BOG	C2-C1-O1-C1'
2	I	219	BOG	C2'-C1'-O1-C1
2	J	218	BOG	C2'-C1'-O1-C1
3	I	218	DMU	C19-C18-O16-C6
2	F	219	BOG	C3'-C4'-C5'-C6'
3	I	218	DMU	C28-C31-C34-C37
2	A	220	BOG	C3'-C4'-C5'-C6'
2	C	218	BOG	C3'-C4'-C5'-C6'
2	K	218	BOG	C3'-C4'-C5'-C6'
3	I	218	DMU	C25-C28-C31-C34
2	A	219	BOG	C3'-C4'-C5'-C6'
2	J	218	BOG	C3'-C4'-C5'-C6'

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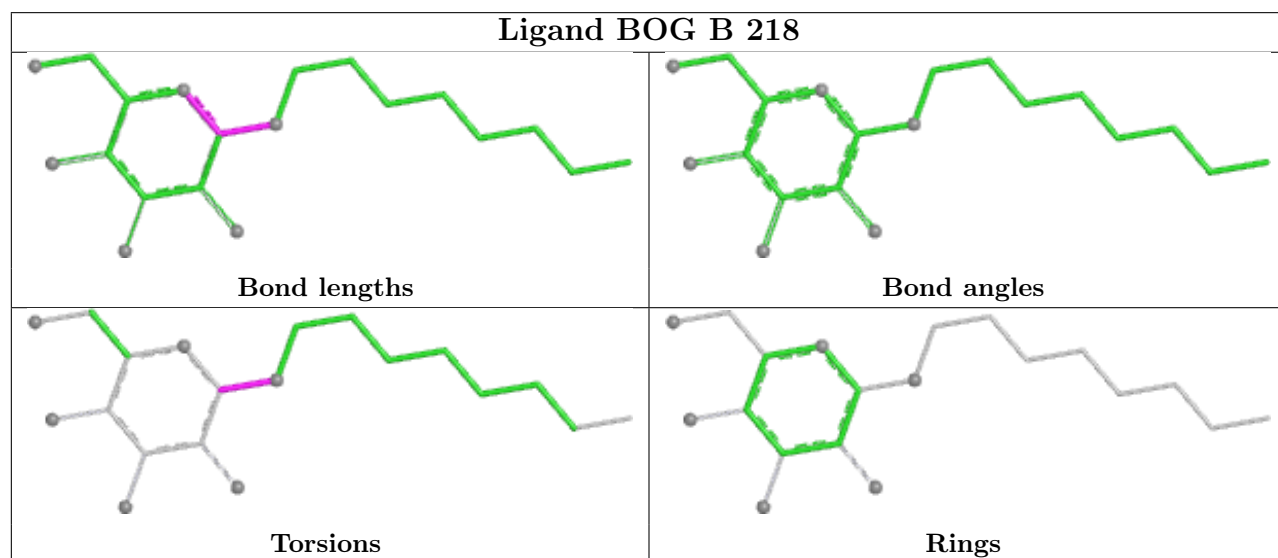
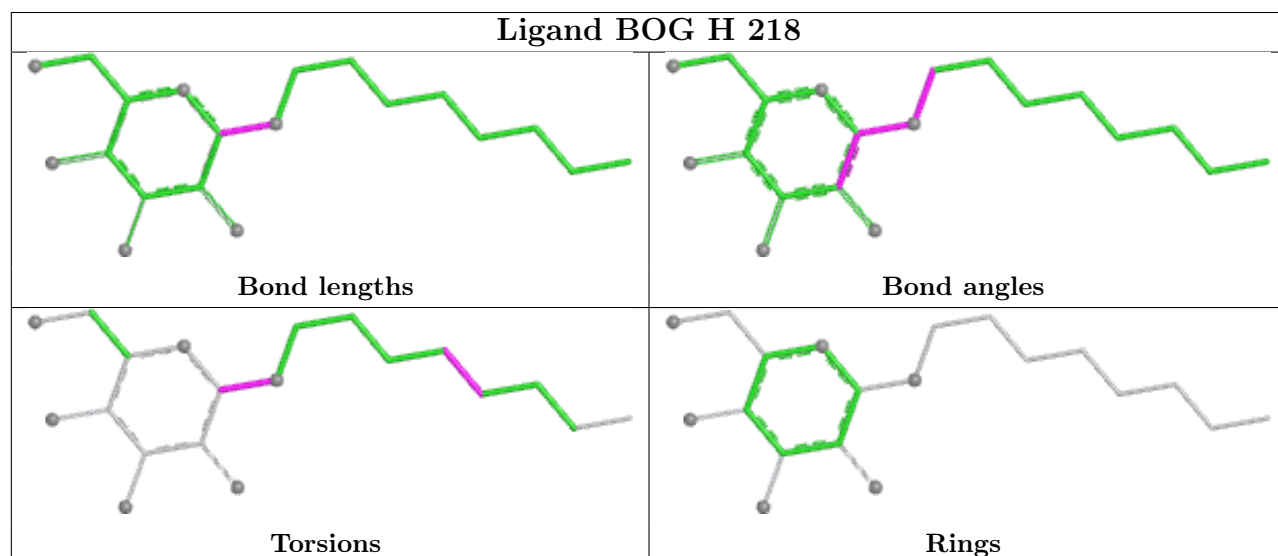
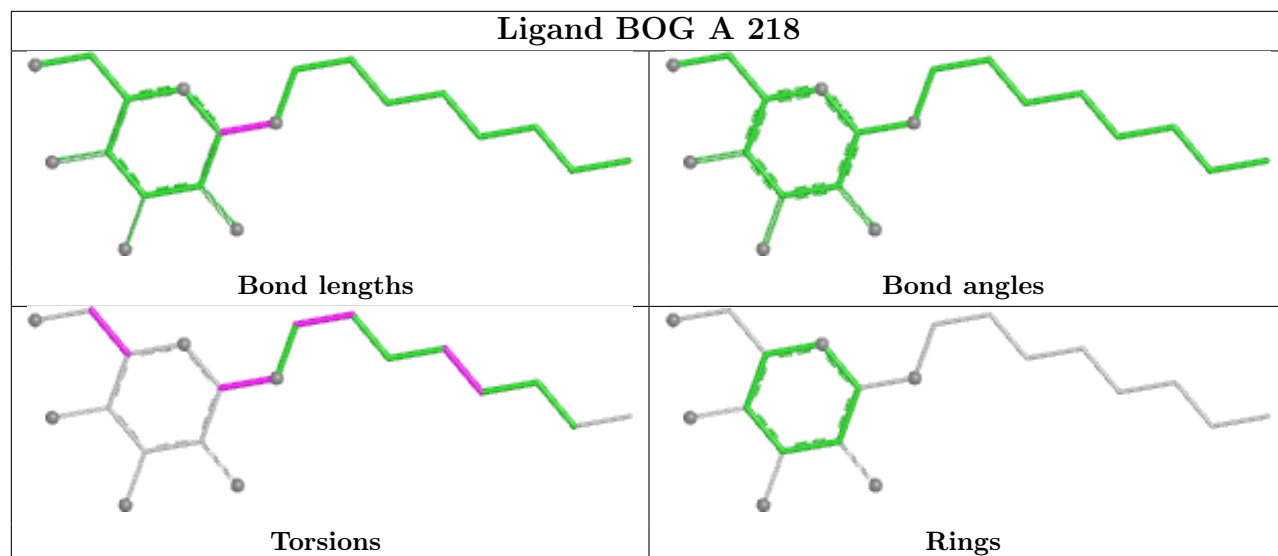
Mol	Chain	Res	Type	Atoms
2	A	220	BOG	O5-C5-C6-O6
3	I	218	DMU	C19-C22-C25-C28
2	I	219	BOG	O1-C1'-C2'-C3'
2	K	218	BOG	C4-C5-C6-O6
2	A	218	BOG	C3'-C4'-C5'-C6'
2	A	220	BOG	O1-C1'-C2'-C3'
3	I	218	DMU	C31-C34-C37-C40
2	C	218	BOG	O1-C1'-C2'-C3'
2	F	218	BOG	C3'-C4'-C5'-C6'
3	I	218	DMU	C22-C25-C28-C31
2	A	218	BOG	O1-C1'-C2'-C3'
2	I	219	BOG	C4-C5-C6-O6
2	C	218	BOG	C2-C1-O1-C1'
2	F	219	BOG	C2'-C1'-O1-C1
3	I	218	DMU	C34-C37-C40-C43
2	K	218	BOG	C2'-C1'-O1-C1
2	H	218	BOG	C3'-C4'-C5'-C6'

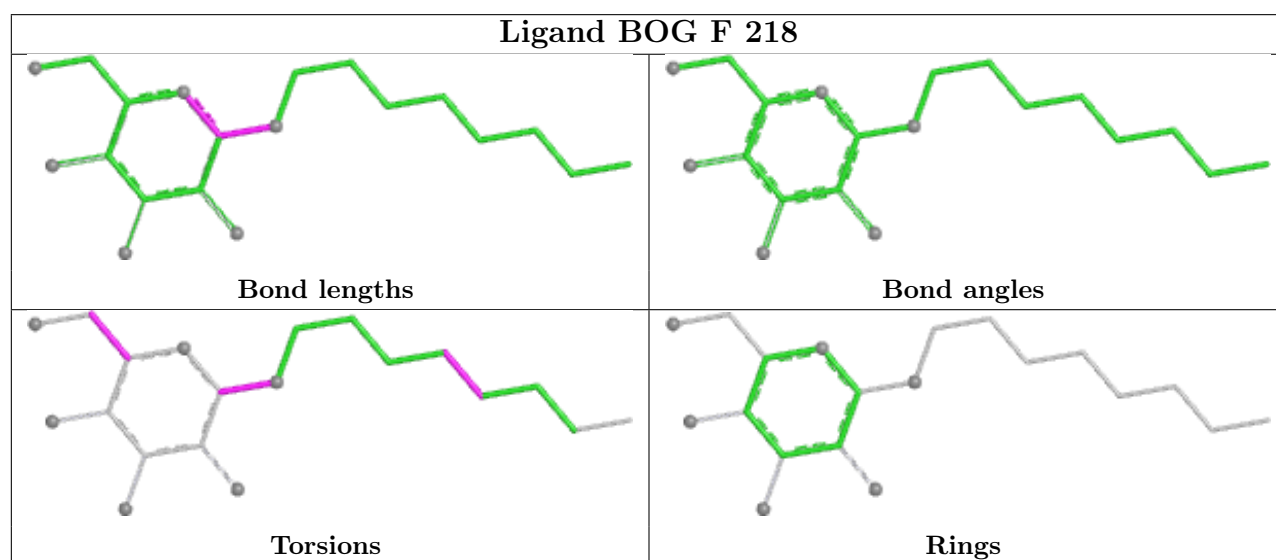
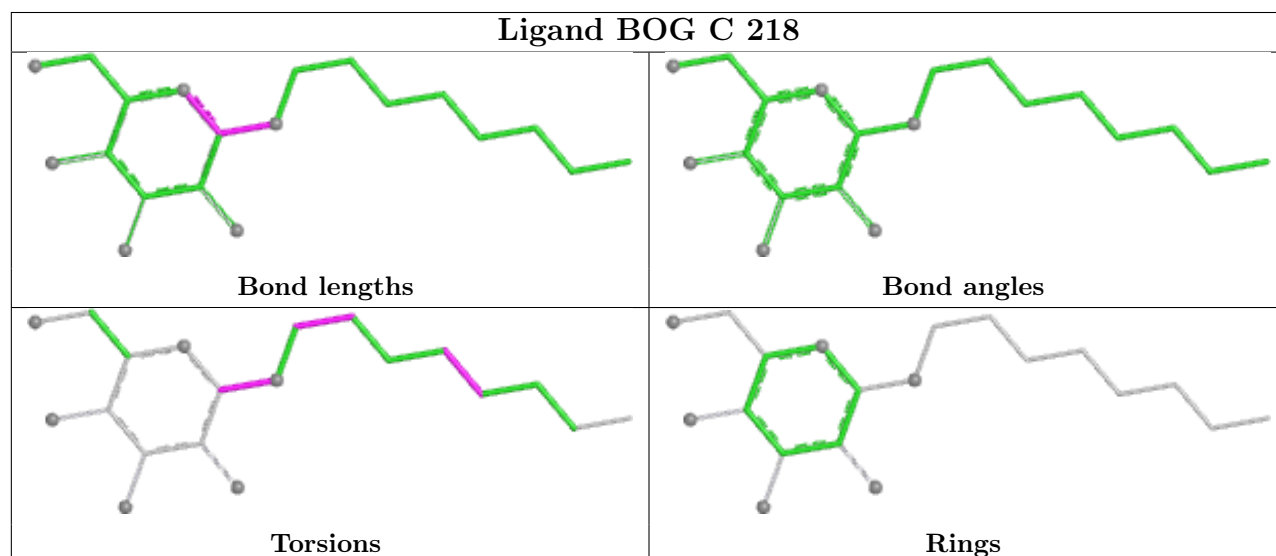
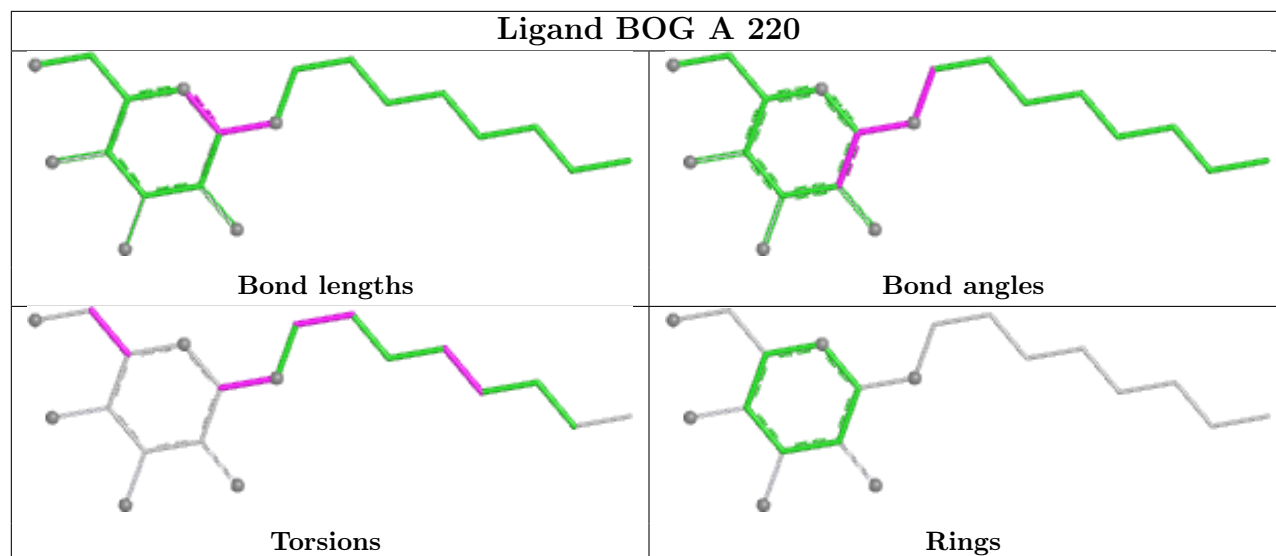
There are no ring outliers.

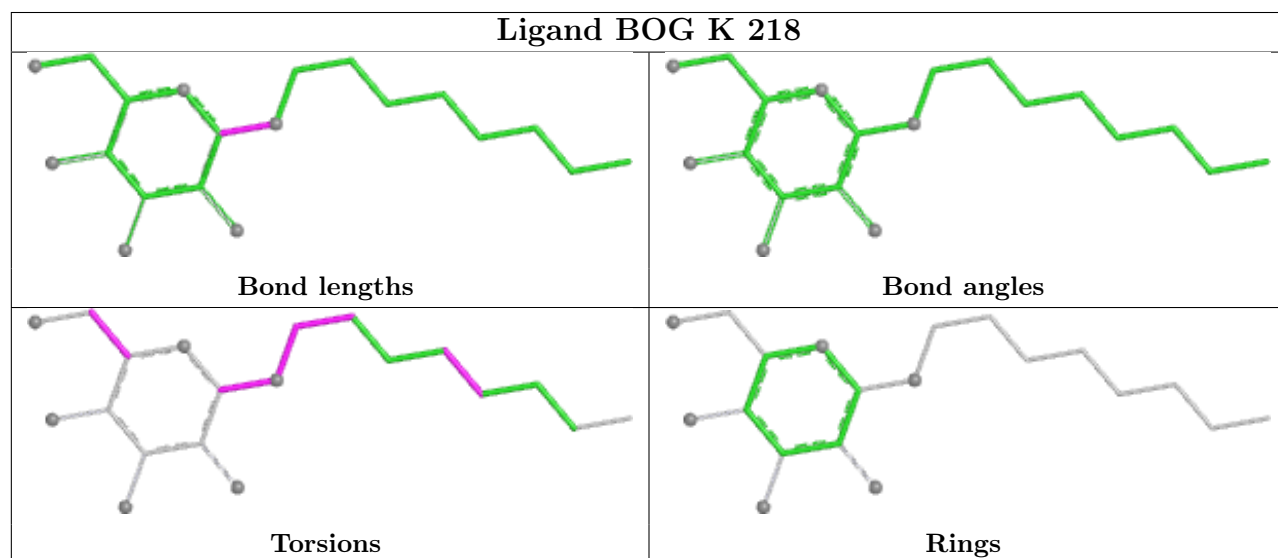
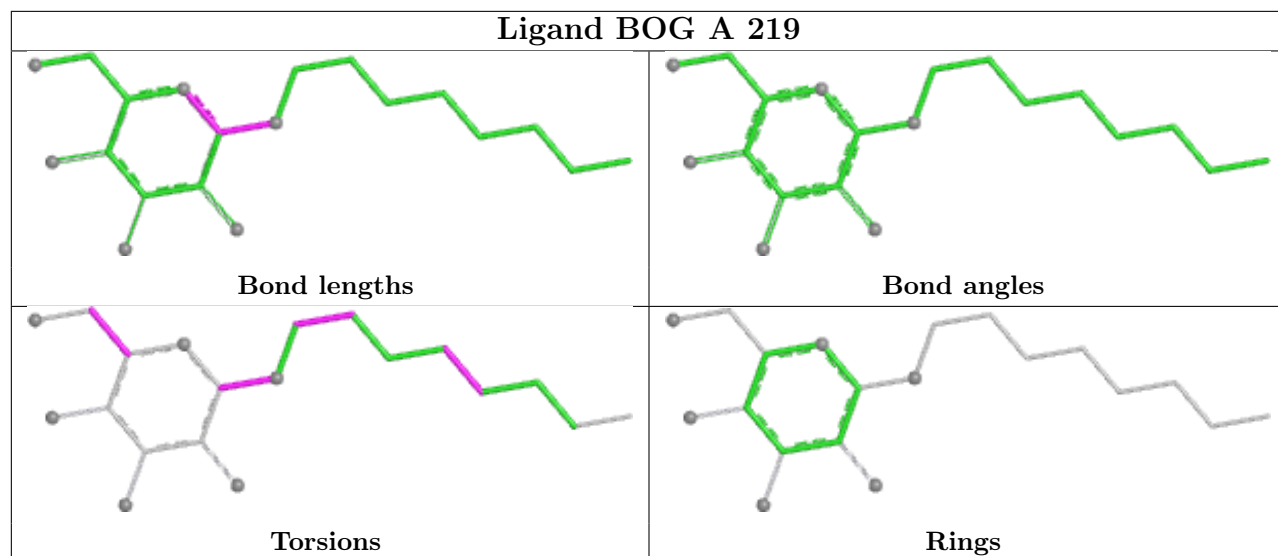
6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	218	BOG	2	0
2	H	218	BOG	4	0
2	B	218	BOG	1	0
2	A	220	BOG	1	0
2	C	218	BOG	1	0
2	A	219	BOG	1	0

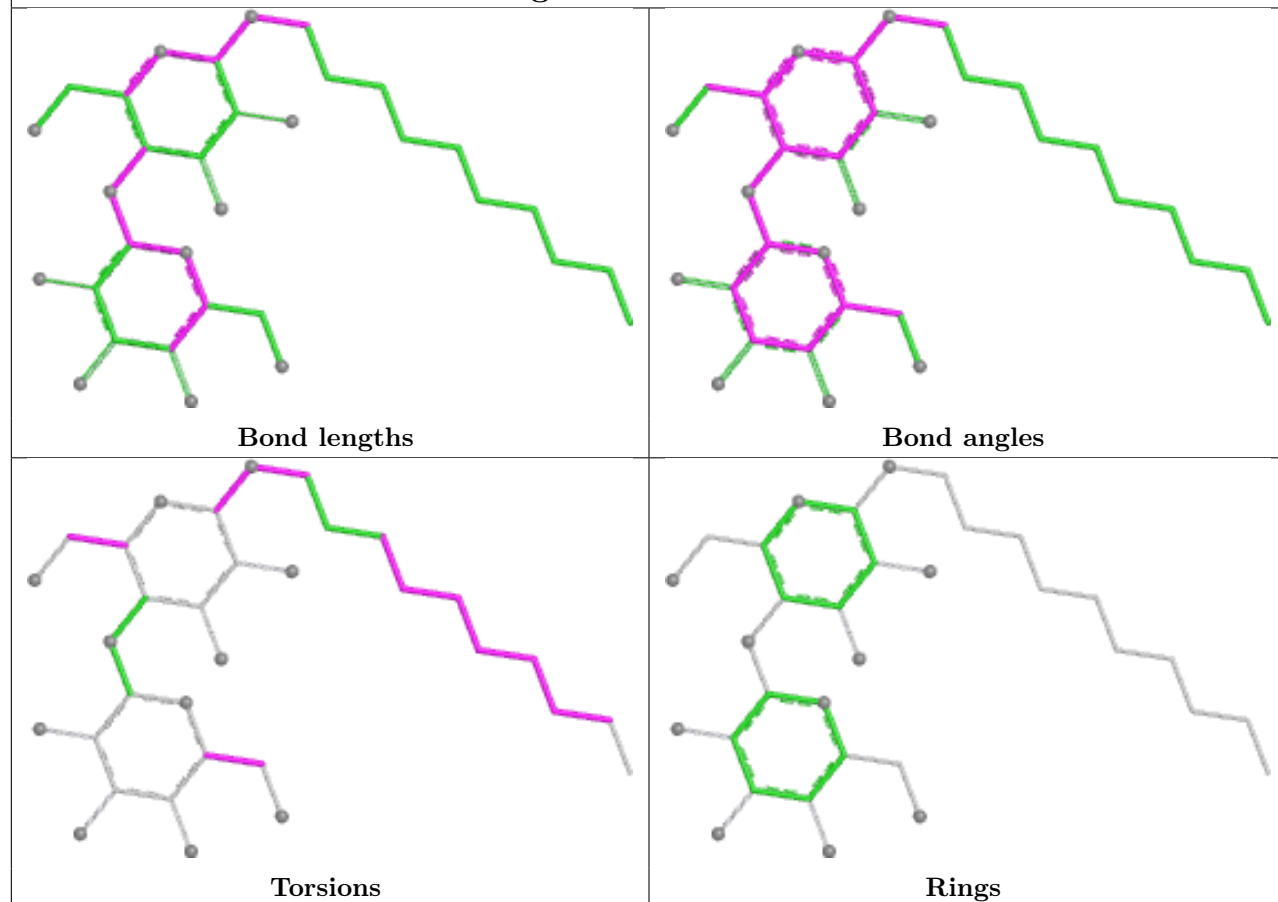
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



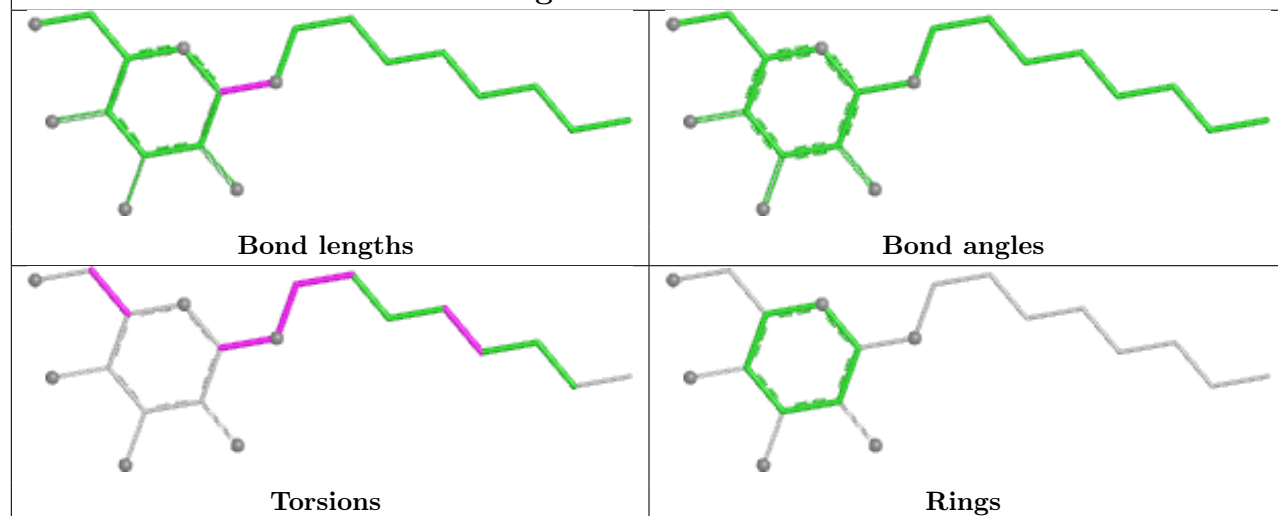


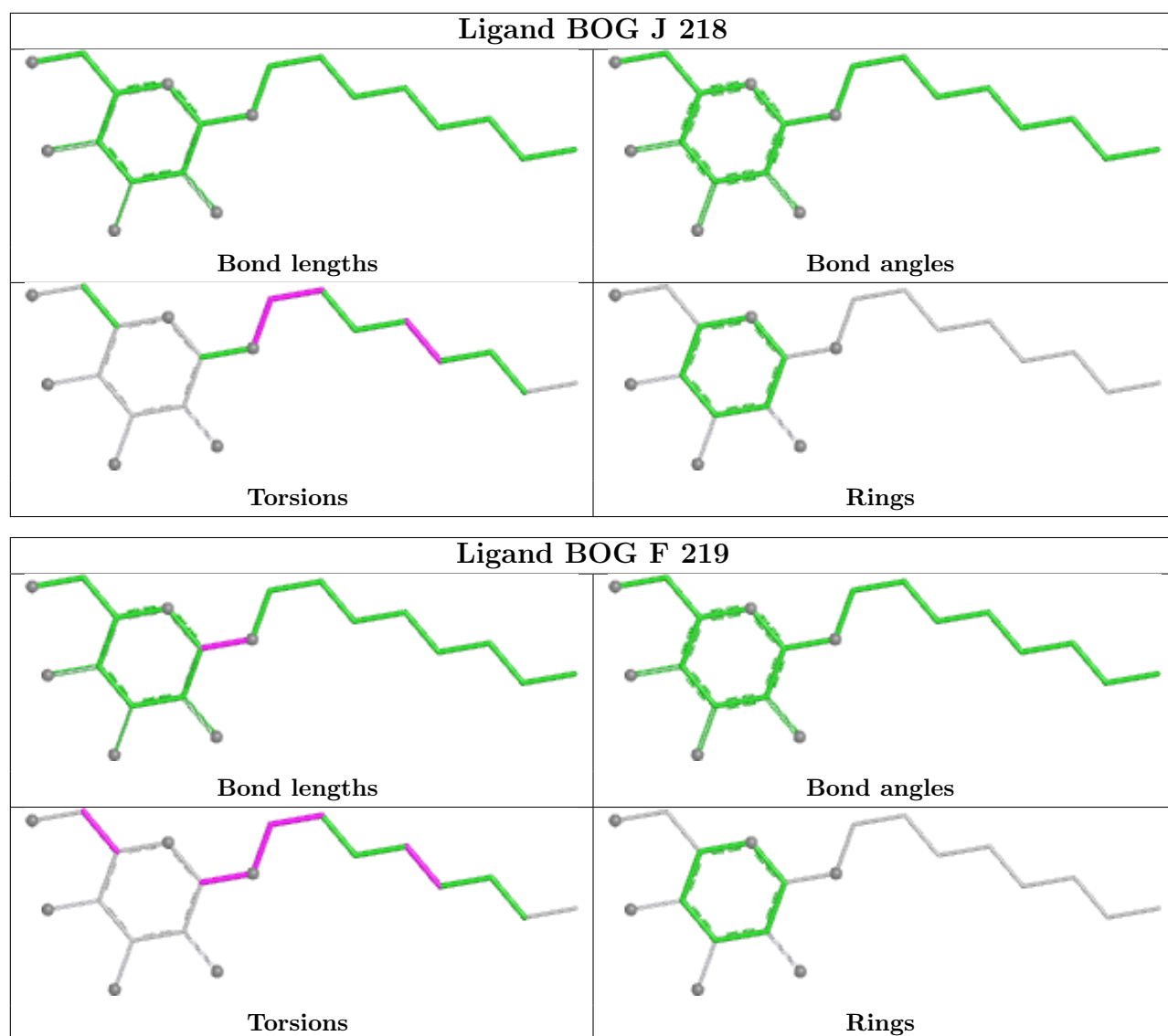


Ligand DMU I 218



Ligand BOG I 219





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	127/128 (99%)	0.32	3 (2%) 59 61	14, 26, 46, 54	0
1	B	127/128 (99%)	0.49	5 (3%) 43 45	19, 31, 42, 47	0
1	C	127/128 (99%)	0.22	2 (1%) 70 72	13, 24, 42, 49	0
1	D	127/128 (99%)	0.52	10 (7%) 18 19	16, 31, 46, 51	0
1	E	127/128 (99%)	0.06	1 (0%) 82 84	14, 22, 35, 42	0
1	F	127/128 (99%)	0.32	2 (1%) 70 72	17, 27, 40, 47	0
1	G	127/128 (99%)	0.31	6 (4%) 36 37	12, 24, 45, 55	0
1	H	128/128 (100%)	0.70	14 (10%) 10 11	15, 30, 48, 53	0
1	I	127/128 (99%)	0.32	5 (3%) 43 45	15, 26, 42, 48	0
1	J	127/128 (99%)	0.49	4 (3%) 51 53	20, 30, 47, 53	0
1	K	127/128 (99%)	0.76	23 (18%) 3 4	18, 31, 60, 65	0
1	L	127/128 (99%)	0.92	13 (10%) 12 13	23, 38, 51, 60	0
All	All	1525/1536 (99%)	0.45	88 (5%) 29 30	12, 29, 47, 65	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	1	GLY	4.5
1	L	103	PHE	4.0
1	G	208	GLY	3.9
1	K	208	GLY	3.8
1	A	174	LEU	3.7
1	G	103	PHE	3.7
1	L	208	GLY	3.6
1	K	207	ASP	3.5
1	C	211	SER	3.4
1	J	119	ILE	3.3
1	H	151	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	H	147	LEU	3.2
1	I	180	ASP	3.2
1	K	174	LEU	3.2
1	A	211	SER	3.1
1	L	149	ASP	3.1
1	C	204	GLY	3.1
1	K	212	LYS	3.1
1	H	149	ASP	3.1
1	H	148	ARG	3.1
1	H	135	LEU	3.0
1	K	214	TRP	3.0
1	K	216	LEU	2.9
1	K	210	VAL	2.9
1	K	213	GLY	2.9
1	H	150	TRP	2.9
1	L	210	VAL	2.9
1	B	153	ASN	2.8
1	L	147	LEU	2.7
1	D	156	ARG	2.7
1	B	120	ALA	2.6
1	H	204	GLY	2.6
1	D	149	ASP	2.6
1	K	217	LEU	2.5
1	L	153	ASN	2.5
1	D	118	LYS	2.5
1	I	204	GLY	2.5
1	K	103	PHE	2.5
1	H	146	PRO	2.5
1	H	157	ASP	2.4
1	B	215	ARG	2.4
1	J	140	VAL	2.4
1	I	103	PHE	2.4
1	K	194	SER	2.4
1	K	193	VAL	2.4
1	D	147	LEU	2.4
1	D	114	ALA	2.3
1	H	118	LYS	2.3
1	K	204	GLY	2.3
1	E	168	SER	2.3
1	D	174	LEU	2.3
1	J	115	LEU	2.3
1	L	157	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	L	180	ASP	2.3
1	K	182	ALA	2.3
1	L	199	GLN	2.3
1	L	109	LEU	2.2
1	D	148	ARG	2.2
1	J	214	TRP	2.2
1	K	201	ILE	2.2
1	I	217	LEU	2.2
1	F	103	PHE	2.2
1	B	148	ARG	2.2
1	K	199	GLN	2.2
1	G	206	ALA	2.2
1	L	168	SER	2.2
1	A	103	PHE	2.2
1	B	180	ASP	2.2
1	H	145	THR	2.2
1	K	148	ARG	2.1
1	F	153	ASN	2.1
1	L	2	SER	2.1
1	K	215	ARG	2.1
1	H	217	LEU	2.1
1	K	203	LEU	2.1
1	I	194	SER	2.1
1	D	115	LEU	2.1
1	K	180	ASP	2.1
1	K	192	PRO	2.1
1	G	210	VAL	2.1
1	D	111	ARG	2.1
1	D	211	SER	2.0
1	G	176	THR	2.0
1	H	142	ASN	2.0
1	L	217	LEU	2.0
1	G	215	ARG	2.0
1	K	211	SER	2.0
1	K	183	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

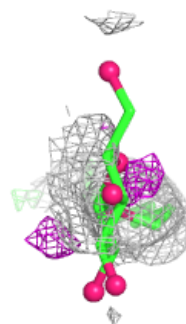
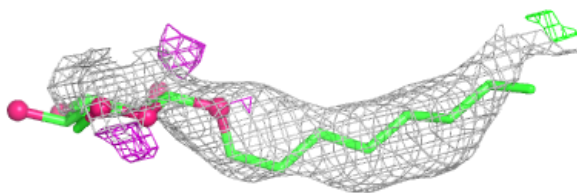
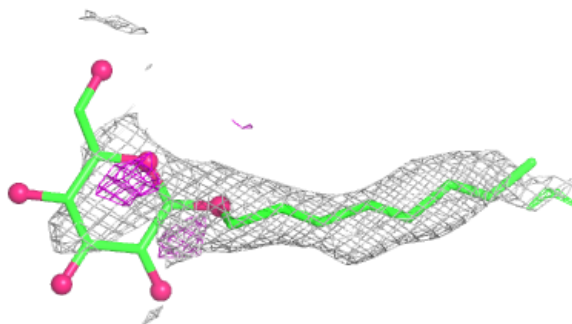
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BOG	H	218	20/20	0.64	0.27	64,77,81,81	0
2	BOG	F	218	20/20	0.72	0.22	53,66,70,71	0
2	BOG	A	218	20/20	0.73	0.21	41,60,65,65	0
2	BOG	J	218	20/20	0.74	0.18	55,65,68,68	0
2	BOG	A	220	20/20	0.75	0.18	55,61,63,63	0
2	BOG	A	219	20/20	0.76	0.20	46,59,63,64	0
2	BOG	B	218	20/20	0.76	0.20	58,61,63,64	0
2	BOG	I	219	20/20	0.76	0.22	48,61,64,65	0
2	BOG	C	218	20/20	0.76	0.20	40,57,63,64	0
2	BOG	K	218	20/20	0.77	0.18	47,58,63,64	0
2	BOG	F	219	20/20	0.78	0.22	58,61,64,64	0
3	DMU	I	218	33/33	0.86	0.12	29,35,38,39	0

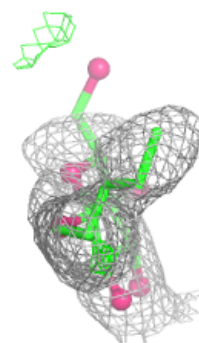
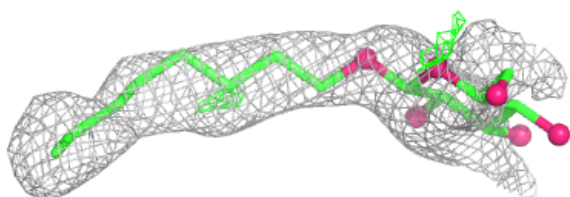
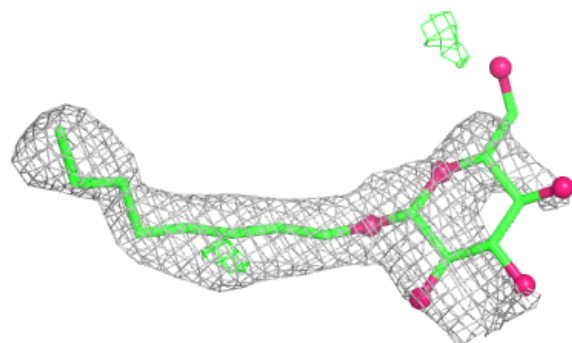
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around BOG H 218:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

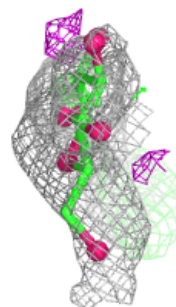
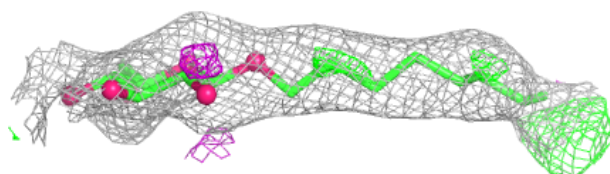
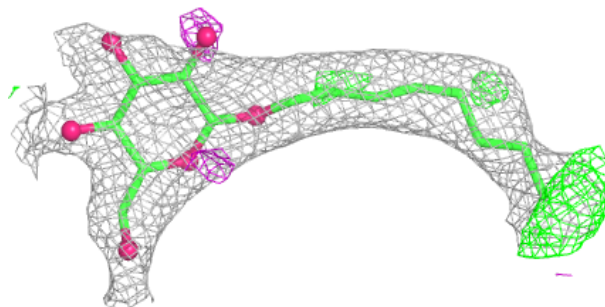
**Electron density around BOG F 218:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

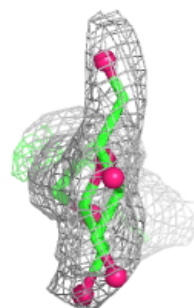
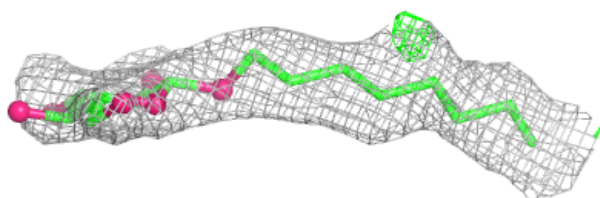
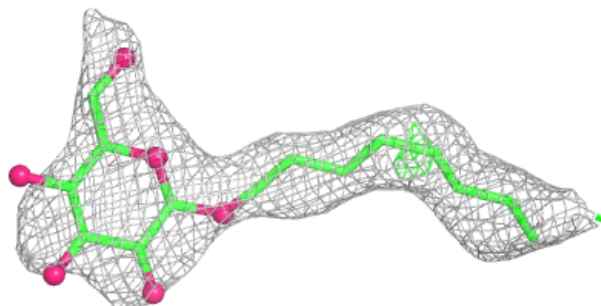


Electron density around BOG A 218:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

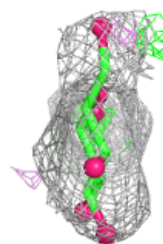
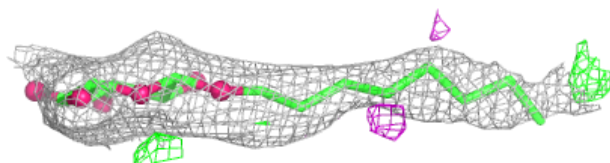
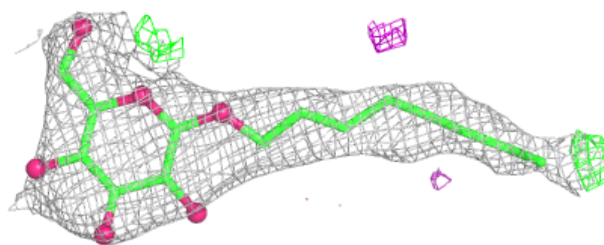
**Electron density around BOG J 218:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

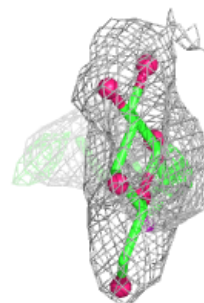
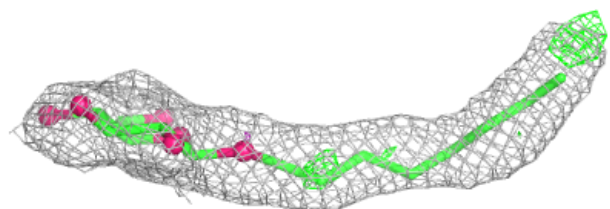
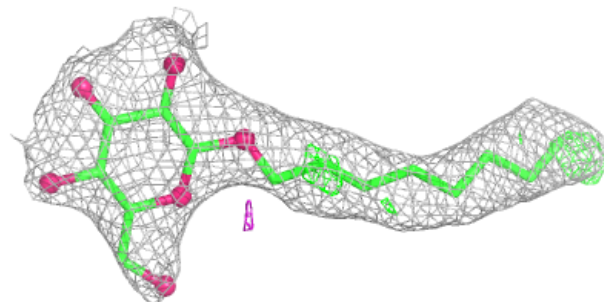


Electron density around BOG A 220:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

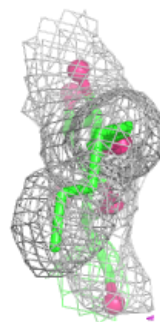
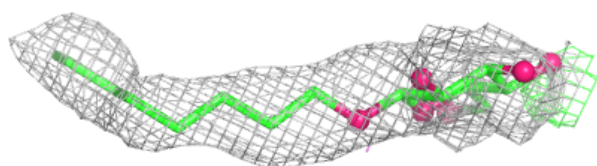
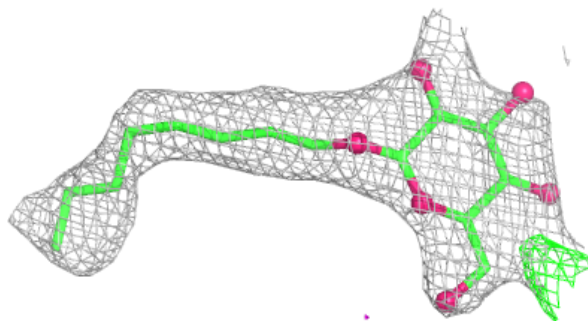
**Electron density around BOG A 219:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

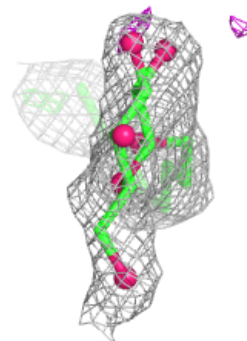
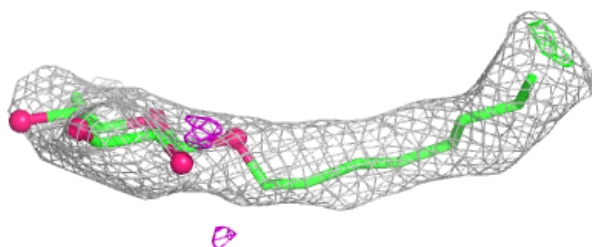
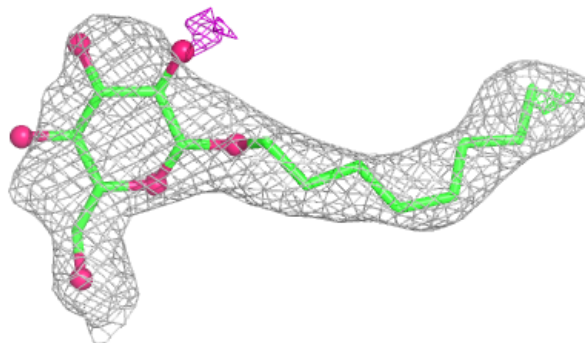


Electron density around BOG B 218:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

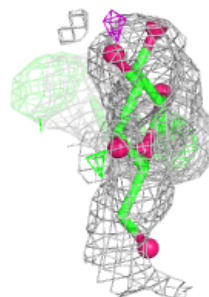
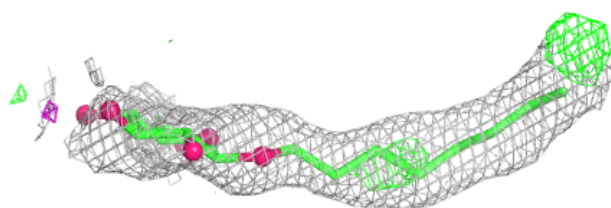
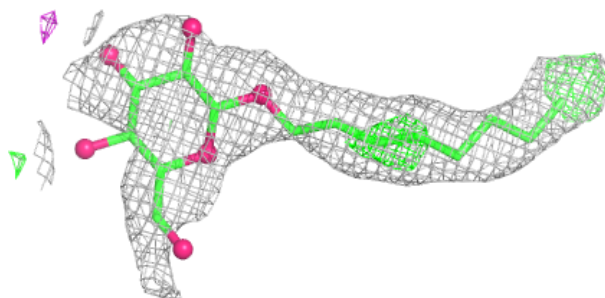
**Electron density around BOG I 219:**

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

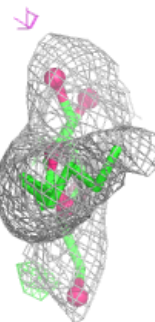
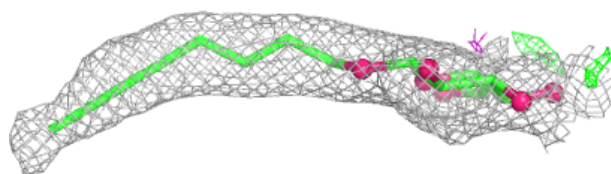
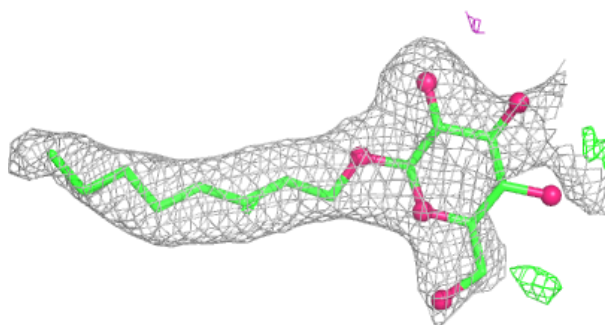


Electron density around BOG C 218:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

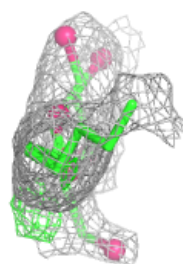
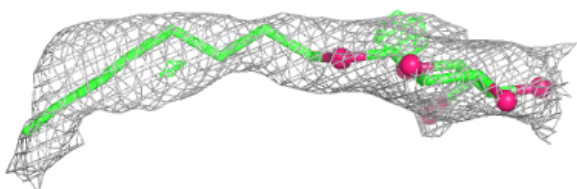
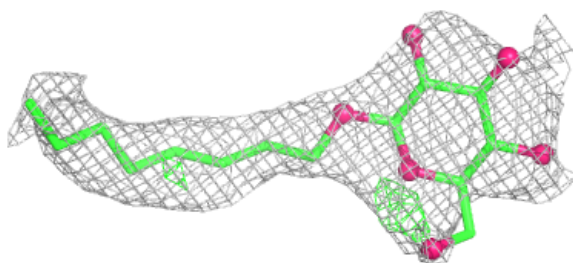
**Electron density around BOG K 218:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

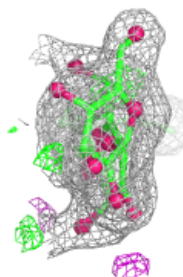
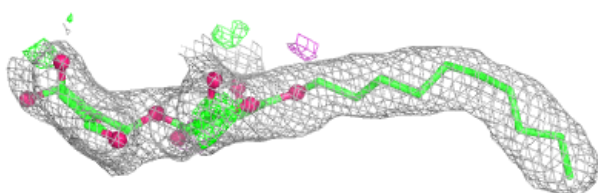
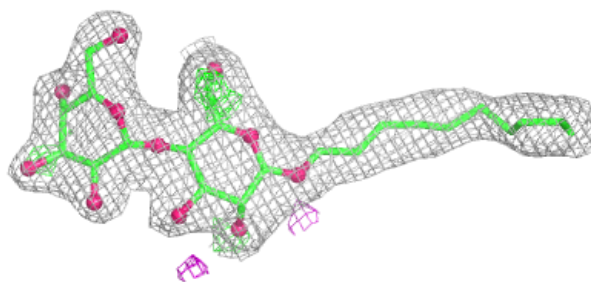


Electron density around BOG F 219:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around DMU I 218:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.